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STUDIES ON THE MODIFIED CLAUS PROCESS: I. EVALUATION OF
CATALYSTS FOR THE $\text{H}_2\text{S}/\text{SO}_2$ REACTION ; AND,
II. CATALYST POISONING IN THE COS/SO_2 REACTION

BY



CHONG - LIEK LIU

A THESIS

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The undersigned certify that they have read, and recommend to the Faculty of Graduate Studies for acceptance a thesis entitled STUDIES ON THE MODIFIED CLAUS PROCESS:

I. EVALUATION OF CATALYSTS FOR THE $\text{H}_2\text{S}/\text{SO}_2$ REACTION; AND

II. CATALYST POISONING IN THE COS/SO_2 REACTION" by

Chong-Liek Liu in partial fulfilment of the requirements for the degree of Master of Science in Chemical Engineering.

ABSTRACT

It is quite well known that bauxite and alumina are active catalysts for the reaction between hydrogen sulfide and sulfur dioxide to form elemental sulfur, but the reason why this is so is still unknown. Seven types of catalysts, namely γ -alumina, 2.0% NaOH-doped γ -alumina, 5.0% NaOH-doped γ -alumina, bauxite, 2.0% NaOH-doped bauxite, H-Y zeolite, Na-Y zeolite, were used to test for their performances towards this reaction and hopefully, from the difference in their chemical constituent, to provide a basis for understanding about the role played by catalyst and thus chemically modifying the catalytic activities. The reactions were all carried out under a same set of conditions (510°K, 1.13 atm and with same feed composition for each catalyst) over a same range of flow rates. It has been found that under the chosen range (similar to the industrial one) of reaction conditions, 2.0% NaOH-doped γ -alumina was most active with H-Y zeolite least active. The sodium doped catalysts were always found to be more active than the undoped counterpart although it was difficult to explain why 5.0% NaOH doped γ -alumina was less active than the 2.0 % NaOH doped γ -alumina. It has been proposed here that sodium ion did play a part in catalyzing the reaction but no strong evidence is yet available to support such assumption.

Another part of the present work was to study the reaction of COS and SO₂ over γ -alumina. The reaction

was carried out in a stainless steel recycle reactor (same as that used in the first part of this work) from 522° to 557°K. It was found that the reaction only proceeded over a short period of time and this was later found due to catalyst poisoning by carbon dioxide, which is the product formed by this reaction. Further investigation by infrared spectrophotometry showed that carbon dioxide was irreversibly chemisorbed on the surface of γ -alumina and thus presumably occupied the sites important for the reaction, which in turn poisoned the catalyst.

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CHAPTER 1

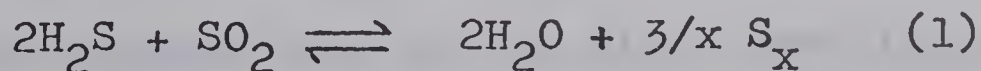
INTRODUCTION

1.1 Feasible Chemical Reactions in Sulfur Recovery Plants

Most of the Claus process sulfur plants treat feedstreams containing hydrocarbon and/or other carbon compounds. In addition to H_2S and SO_2 , other components such as COS , CS_2 , CO_2 and H_2O can appear in the stream leaving the waste-heat boiler and entering the catalytic converter. To improve catalytic converter design by including all important chemical steps, it is necessary to examine the feasibility of the various reactions which may occur. Those reactions which are demonstrated to be thermodynamically infeasible can be ignored in carrying out reactor design. A free energy minimization method was used to evaluate the thermodynamic equilibria in the present study.

1.2 Modified Claus Process for Production of Elemental Sulfur

The major step in the modified Claus reaction,



for producing elemental sulfur has been discussed extensively in the literature. The most generally used cata-

lysts for this Claus reaction are bauxite and alumina however, many investigators have studied other catalysts to increase the conversion of H_2S and SO_2 to elemental sulfur. A detailed review of the Claus reaction as well as the catalysts which have been used will be presented in section 2.1 of the literature survey.

Gamson and Elkins [30] carried out kinetics measurements of the Claus reaction over alumina catalyst in an integral reactor at a temperature of 230° to 300°C over four rather low space velocities. Cormode [20] used Porocel (a commercial bauxite catalyst) to obtain kinetic data for the Claus reaction in a recycle flow reactor in the initial investigation of this program at the University of Alberta. McGregor [53] carried out a series of 80 experimental runs in a similar but improved reaction apparatus, performed at four different temperatures (between 481 and 560°K) and at varying partial pressure of H_2S , SO_2 and H_2O to obtain the rate equation and activation energy for the forward step in the reversible Claus reaction. Water vapor was found to have a retarding effect on the forward rate of the Claus reaction as its concentration increased.

1.3 Objections of this Research Project

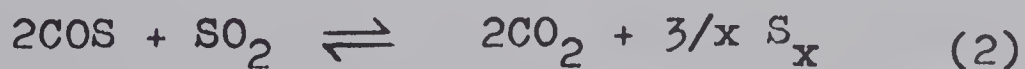
1.3.1 To Evaluate Alternative Catalysts for Reaction between H_2S and SO_2

Although many past investigators have tried to develop more active or more efficient catalysts for the reaction between H_2S and SO_2 and many innovations have been patented, a systematic comparison of industrial catalysts under standardized reaction conditions does not appear in the chemical literature. Most of the previous works were aiming at improving the physical properties of the catalysts by increasing the catalyst specific surface area or by modifying the physical structure of the catalysts. It has been shown that elemental sulfur, formed from Claus reaction, can plug up the micropores of the catalyst [51] and in turn eliminate a large portion of the available surface area. Hence, the object of developing a larger specific area may be pointless. Rather, studies of the chemical properties of catalysts towards improving the catalytic activity for the reaction between H_2S and SO_2 might be more rewarding. So far, no clear evidence regarding the "source" of the catalytic activities seems available.

As a result, the present studies were designed to make a comparison of some industrial catalysts under a same range of reaction conditions similar to the industrial ones over a short term reaction period and perhaps, from the difference in chemical constituents of these catalysts, to provide a basis for understanding and thus hopefully chemically modifying the catalytic activities. The catalysts used were bauxite, γ -alumina, H-Y zeolite, Na-Y zeolite, 2.0 % NaOH-doped γ -alumina, 5.0 % NaOH-doped γ -alumina and 2.0 % NaOH-doped bauxite.

1.3.2 To Measure the Kinetics for the Reaction between COS and SO₂

Much of the losses from sulfur plants can be attributed to sulfur-bearing gaseous constituents such as COS and CS₂ [70]. From a thermodynamic study by Gamson and Elkins [30], it was found that the equilibrium conversion of the following reaction



was higher than that of the reaction between H₂S and SO₂. Gamson and Elkins [30] also carried out a kinetics study of reaction (2) over γ -alumina catalyst at temperatures from 230°C to 300°C at four rather low flow

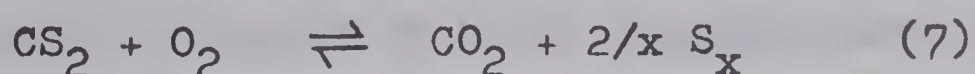
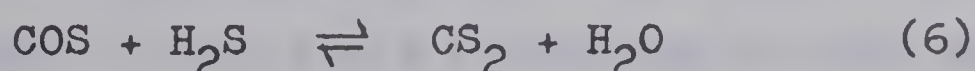
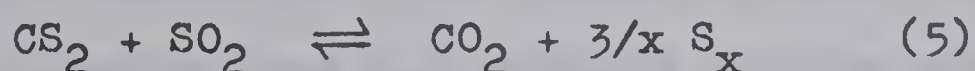
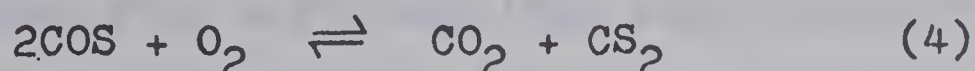
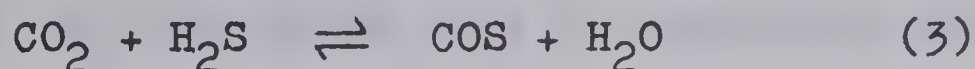
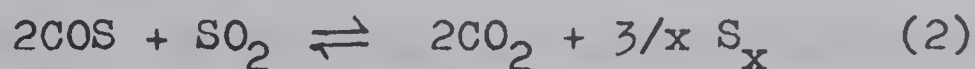
rates in an integral reactor. The conversion was found to range from 64 % to 96 %. Owing to the high feasibility of this reaction shown by past investigators, kinetics measurements and mechanistic studies of this reaction over γ -alumina from 522°K to 557°K were carried out in the present work to provide information which hopefully will be of value in reducing sulfur losses.

In all of the studies on this reaction done by past workers, nothing was mentioned about the attainment of steady activity of catalysts. In the present studies, reaction was allowed to proceed long enough so that its short-term activity could be stabilized.

CHAPTER 2

LITERATURE SURVEY

In Claus process sulfur plants, side-reactions may occur in furnaces and waste-heat boilers to produce appreciable quantities of COS and CS₂ from CO₂ and hydrocarbons [12, 13]. Zawadski et al [98] showed that between 800° and 850°C, methane reacted with SO₂ to form large quantities of COS and CS₂. Opekar and Goar [61] suggested that some of the following reactions might occur in catalytic converter,



Although the present work is mainly concerned with a comparison of activities of different catalytic agents for the reaction between H₂S and SO₂ or with the kinetics studies of the reaction between COS and SO₂, this literature survey also covers other reactions which supposedly proceed in parallel in the catalytic converter. This background should provide a clearer

picture of the reactions which occur in sulfur plants and what can be understood about them.

2.1 Catalytic Reaction of H_2S with SO_2

The reaction of H_2S and SO_2 in the presence of water was a common lecture room demonstration as early as 1812. Cluzel [18] noted at that time that no combination would result if the gases were first dried by passing over calcium chloride. Udintseva and Chufarov [88] found that H_2S and SO_2 would not react homogeneously between 250° and $350^\circ C$. In the original process developed by Claus [17] H_2S was mixed with the necessary amount of air and passed over a red hot iron oxide catalyst. Dry bed catalytic conversion first became a commercial process for sulfur recovery from H_2S produced in coke oven between 1883 and 1887. Large scale processing of sour gas and effective sulfur recovery did not commence until the 1940's with the operation of the gas processing unit at McKanick, Arkansas by the Arkansas Fuel Oil Company.

From the literature, it was found that most of the catalysts used for the reaction between H_2S and SO_2 were sulfides and oxides of aluminum and other transition elements. More commonly studied ones were iron oxide, bauxite, titanite iron, manganese dioxide, alumina, glass, aluminosilicates.

silicate, silver, silver sulfide, cobalt sulfide, molybdenum sulfide, cobalt molybdenum-alumina, cobalt thiomolydate, and glassy alkalized alumina. Besides these, activated carbon was also very popular.

Iron oxide was the catalyst studied by Claus himself [17]. Bauxite is one of the most generally used catalysts in present-day Claus sulfur plants. Petrumic [66] reported that bauxite catalyst of 2/4 mesh size proved to be lacking in mechanical strength and varied physically and chemically from shipment to shipment. Projahn [68] also investigated the properties of bauxite. Fundamental works on the kinetics of sulfur production from H_2S were carried out by Prettre and Sion [67] using aluminosilicate as catalysts and these catalysts were found to adsorb SO_2 more readily so that the concentration of H_2S was believed to determine the rate of the reaction. Gamson and Elkins [30] studied the kinetics of the reaction between H_2S and SO_2 in an integral bed reactor using alumina as catalyst. Heinemann et al [37] concluded from their work that it seemed evident that the high Claus activity of bauxite or alumina catalysts was usually found to coincide with their good desiccant properties. Projahn [68] used titanitic iron oxide, Tyers and Hedley [88] used titanium salts, and Carpenter and Linder [13] used manganese oxide as catalysts.

Taylor and Wesley [77] studied the Claus reaction over Pyrex glass surface and found that overall reaction rates were proportional to the glass surface area. A rate equation of the form,

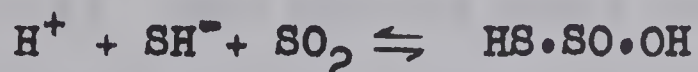
$$-r_{H_2S} = k A_E P_{H_2S}^{1.5} P_{SO_2}$$

where A_E is the surface area of glass, for the conversion of H_2S had been proposed. They also reported that no measureable homogeneous reaction took place at $580^\circ C$.

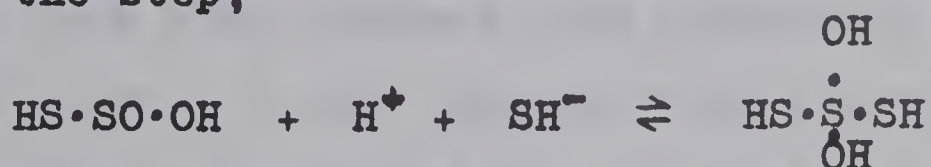
Sanjiva et al [71] found an autocatalytic reaction over silver catalyst and this was explained by the fact that silver sulfide was first formed from the reaction, then silver sulfide in the presence of water is a very active catalyst for the reaction between H_2S and SO_2 . Murthy and Rao [55] studied the Claus reaction by using some metallic sulfides like cobalt thiomolybdate, cobalt sulfide and molybdenum sulfide, as catalysts in a batch recycle reactor and found that at $25^\circ C$, the reaction would not proceed with any of their catalysts unless water was present. It was postulated that the reaction took place in the following sequential steps,



Activated carbon was used as a catalyst by Naeff [57] and Prettre and Sion [67]. By using cobalt-molybdenum-alumina catalyst mixture, Hammar [35] proposed the following mechanism for the Claus reaction. Primarily, SO_2 and H_2S were adsorbed on adjacent active sites of the catalyst. H_2S dissociated into H^+ and SH^- and hence the reaction

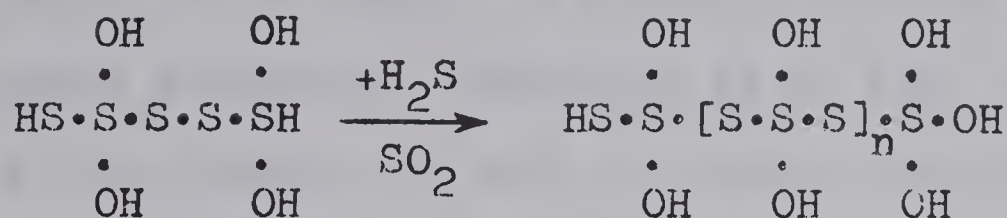
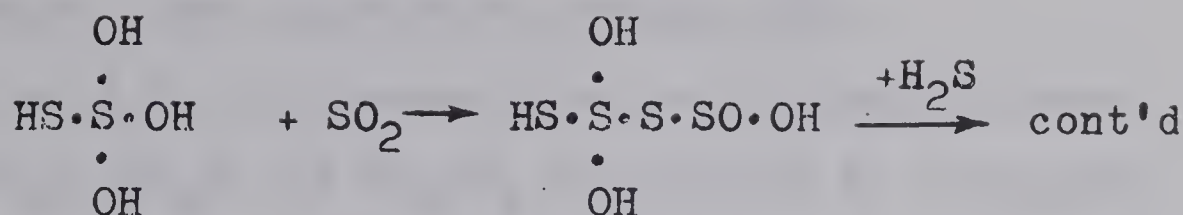


took place. He could not suggest how the intermediate reacted further, but offered two possibilities. One case involved the step,



whose product permits water to split off and sulfur, in the form of S_3 , adsorbs on the catalyst.

The other possibility involved,



Water is split off from all of the intermediates at different rates and the sulfur formed will be distributed according to some probability function.

2.2 Catalytic Reaction of COS with SO₂

Formation of elemental sulfur was observed by Caddick [11] when COS was mixed with an excess of SO₂ and passed over red hot pumice or brick. Avdeeva [3] also studied the reaction between COS and SO₂ and best results were obtained at 400° to 425°C over a catalyst prepared from blast furnace slag containing about 55 % aluminum oxide. It was believed that the oxide added to the mechanical strength of the catalyst but did not improve its activity and the presence of iron decreased both the catalyst strength and activity. Udintseva and Chufarov [87] investigated the reaction at 600° to 800°C in the presence of oxides of iron, aluminum, or titanium on pumice and porcelain supports. It was found that

reaction ceased when conversion reached 90%.

Gruvaktiebolag [34] discovered that such alkaline compounds as Na_2O , Na_2S and Na_2CO_3 functioned as catalysts at temperatures above 350°C either in aqueous solution or deposited on a porous supports. Chowdhury et al [16] and Gamson [29] found that bauxite is also an active catalyst for this reaction. Wallden and Ruth [89] proposed to recover sulfur from COS by oxidation with sulfur dioxide below 350°C . Griffith and Hill [33] used nickel subsulfide as catalyst to study the oxidation of COS by oxygen and SO_2 . They found that SO_2 had a retarding effect on the oxidation of COS by O_2 .

Lepsoe [45] conducted an experiment of the homogeneous reaction between COS and SO_2 in an integral reactor and found that the reaction proceeded very slowly even at 800°C , but almost any kind of hot surface was capable of catalyzing the reaction at this temperature. He also found that run-of-mine pyrrhotite was efficient at 700°C and at lower temperature, alumina, in various slightly hydrated and acid soluble forms (boehmite) was a remarkably efficient catalyst; lightly calcined Guiana bauxite and activated alumina were also both satisfactory. In addition to these, alumina was employed as a catalyst on a carrier of porous cement or it might be sintered to crushed firebrick by means of a binding agent such as

sodium silicate. He suggested that although no detailed investigations regarding the catalyst mechanisms had been made, in all probability, surface compounds of SO_2 and the catalysts were formed. The pronounced adsorption of SO_2 was manifested by the way the catalyst tenaciously retained SO_2 once it had been exposed to concentrated SO_2 gas mixtures. The efficiency of the alumina catalysts was found to be partly lost after they were exposed to high temperature for long period of time in his works. In the range of 300° to 600°C , the reduction of SO_2 by COS was reported to be a reaction of first order.

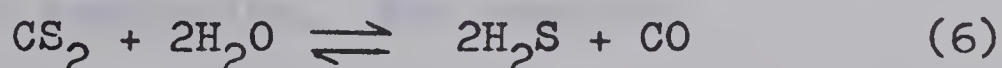
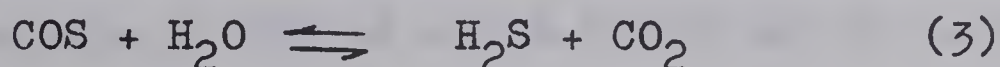
Gamson and Elkins [30] studied the reaction between COS and SO_2 over bauxite catalysts in an integral reactor and found that with a gas stream composition of 5.5% COS, 2.75% SO_2 and 91.75% N_2 (volumetric basis) yields of 90% or better were attainable between 250 and 300°C at a space velocity of 200 std cu ft / (cu ft cat.)(hr). A typical sulfur plant space velocity falls between 650 and 900 std cu ft / (cu ft cat.) (hr) [19] and so conversion for such reaction may be limited in commercial bauxite converters by the short contact time.

In all the previous works in the literature, nothing was reported on the attainment of steady activity of the catalyst when the data of the reaction between COS and SO_2 were collected.

2.3 Simultaneous Catalytic Reactions

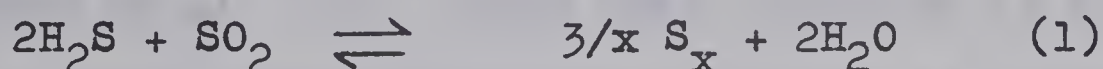
2.3.1 Hydrolysis Reactions

Cameron and Beavon [12] suggested a means of CS_2 and COS removal by the following reactions



Thompson et al [84] found that the reaction of COS with H_2O closely followed a unimolecular path and was catalyzed slowly by many substances and ions, especially by hydroxyl ion. Klason [41] and Schulze [74] found that because both H_2S and SO_2 are acidic, COS was relatively stable towards acids. It existed indefinitely in an aqueous solution containing 50 wt % H_2SO_4 . Dewar and Cranston [24] found that COS decomposed to H_2S in carbonated mineral waters after long storage in closed containers. Although hydrolysis was noted to be accelerated by alkaline materials, COS was still only slowly hydrolyzed by strongly alkaline reagents, such as sodium hydroxide [5]. Heinemann [36] noticed that COS present in a petroleum naptha was hydrolyzed to H_2S by contact with activated bauxite at 370°C . Ferm [26] could dry liquefied petroleum gas containing COS by silica

gel without affecting the COS. Hence silica gel may not be a catalyst for hydrolysis of COS. Sawyer et al [73] reported that in Matheson's Mckemie plant, the two converter stages were maintained at different temperature levels. The principal reaction in the first converter was hydrolysis of COS at about 750°F and it went essentially to completion. The reaction



took place in the second converter at 450 ° to 500°F. Namba and Shiba [58] used 8 to 20 mesh Al_2O_3 to study the kinetics of hydrolysis of COS and CS_2 at a temperature range of 220° to 330°C. The rate of hydrolysis in both cases was first order with respect to COS or CS_2 . The activation energy of hydrolysis of COS was 2.9 Kcal/mole and that of CS_2 was 9.6 Kcal/mole. Other workers who also studied the hydrolysis of CS_2 were Bacon et al [4] and Thacker et al [80]. Buchback [10] suggested that hydrolysis of COS occurred in two steps



2.3.2 Oxidation Reactions

Oxidation of H_2S , COS and CS_2 by air occur in the furnaces and waste heat boilers of sulfur plants. Pan American catalytic direct oxidation process [32] produces sulfur by direct oxidation of H_2S with air. Although elemental sulfur can be produced by catalytic oxidation of H_2S , oxygen will also react with elemental sulfur. Sawyer et al [73] found that oxidation of H_2S occurred at a lower temperature than oxidation of elemental sulfur. In Claus process, a respectable yield of sulfur was obtained by maintaining furnace temperature at sufficiently low levels. Levy and Merryman [46, 47, 48, 49] investigated the kinetics and mechanisms of the combustion of H_2S --air mixtures using a mass spectrometric flame technique. They noted two distinct reaction zones from oxidation of COS in low pressure (0.1 atm); a zone in which CO and SO_2 were formed and a zone in which the CO oxidation was complete. Rate of COS oxidation was measured and a rate equation,

$$-d(\text{COS})/dt = k(\text{COS})(\text{O}_2)$$

was proposed. It was also suggested that the initial step of oxidation was the abstraction of a sulfur atom by an oxygen molecule,

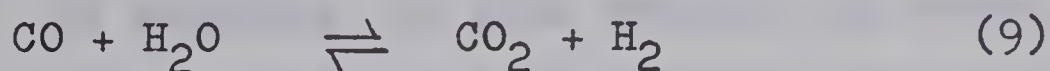
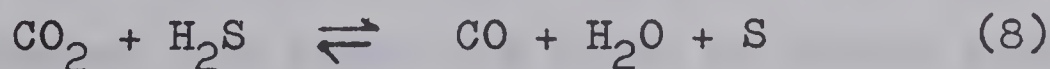


The rate constant was found to be $8.2 \times 10^{14} \exp(-29,100/RT)$ c.c. mole⁻¹sec⁻¹. Griffith and Hill [33] studied the oxidation of COS and CS₂ by air in a glass tube at temperatures above 140°C and noticed that the non-explosive oxidation of CS₂ occurred with simultaneous production of ozone. This homogeneous oxidation was difficult to suppress. The heterogeneous oxidation over nickel sulfide was only possible after the addition of small amounts of ethylene to the reactants. The heterogeneous reaction behaved zero order with respect to CS₂. However, they found that COS did not undergo homogeneous oxidation so readily, and no difficulty existed in experimenting with the heterogeneous reaction alone. The rate of oxidation of COS was retarded by SO₂ and was first order with respect to COS. Information concerning the explosion of mixtures of oxygen with CS₂ and COS can also be found from work done by Thompson [81,82,83]. Isothermal oxidation of CS₂ and COS was conducted by Homann et al [38]. Caddick [11] found that the combustion of CS₂ with an insufficiently supply of oxygen yielded a mixture of unchanged CS₂, CO₂, SO₂, and CO. Kondratiev [42] studied the cold flame oxidation of CS₂ and reported the final products to be CO, SO₂, and some COS. An investigation of

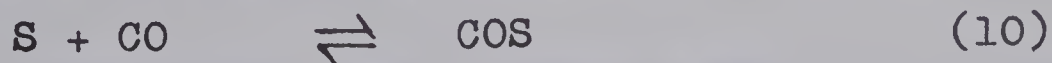
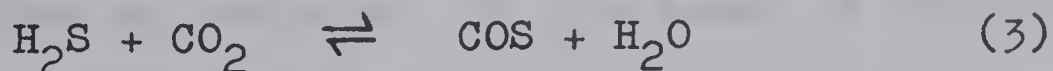
the combustion of COS and CS₂ in rarefield flames at 500°C using spectral and EPR techniques by Sarkisyan and Nalbandyan [72] showed that SO and O were present in both cases

2.3.3 Reactions of Some Sulfur Compounds with CO₂ and/or CO

Caddick [11] passed a mixture of CO₂ and H₂S over a tube containing red hot pumice or red hot brick and found that CO and H₂ were always formed. Reaction occurred to a greater extent in the presence of platinized quartz. The following reactions were suggested to be taking place,

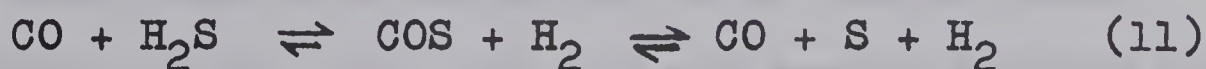


Sawyer et al [73] studied the furnace reaction at 1000°C in the Matheson Process and believed that the formation of COS may be due to the following reactions,

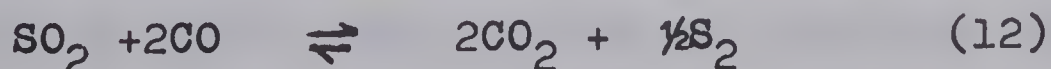


They disagreed with Caddick's view that reaction (8)

occurred. This was explained by the fact that during furnace operations, CO_2 disappeared at a rate faster than its reduction by H_2S to form CO, elemental sulfur and water. In addition, only a small amount of CO was detected in the furnace exit gas. Caddick [11] passed equal volume of CO and H_2S over red hot pumice and found that over 11 % of the final gas was H_2 . The following reaction was suggested to occur



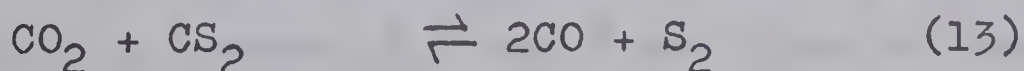
In the same experiment, traces of free hydrogen were detected when H_2S alone was passed through the catalyst. When the tube was packed with platinized quartz in place of pumice, dissociation of H_2S was at first thought to be more pronounced, but later was found to remain very limited in extent. In addition, he also studied the reaction between CO_2 and SO_2 and found that at most only small quantities of CO were formed. Lepsoe [45] carried out the reduction of SO_2 by CO over alumina catalyst in the temperature range of 300° to 600°C and obtained CO_2 and elemental sulfur as products. In his study of reduction of SO_2 by coke, the reaction,



was also believed to proceed with a reaction order of one

over the surface of the coke with ash as catalyst.

Caddick [11] also performed a series of catalytic reactions between CO_2 , CS_2 , H_2O and S. For the reaction of CO_2 and CS_2 , he found that CO was formed in varying amounts according to the reaction conditions. Platinized quartz catalyst, high temperature and high concentration of CS_2 were all favourable to the production of CO. As much as 40.7 % of CO_2 was in one case reduced to CO. The following reactions were suggested to be taking place when a mixture of CO_2 , CS_2 and H_2O was passed through the red hot pumice



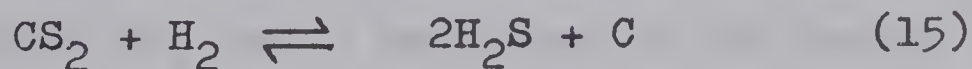
When sulfur vapor was used in place of H_2O , 2.6 % of CO_2 was converted to CO. More than 10 % of the CO_2 could be reduced if sulfur vapor was omitted. Yushkevich et al [94,95,96,97] studied the reaction of SO_2 with CO and H_2O over iron-alumina catalyst. Within the temperature range of 500° to 800°C , the reaction was complete but the yield of sulfur was only 40 to 60 %, the rest being H_2S

and CO_2 . The formation of COS and CS_2 was said to be negligible at 400° to 800°C . Reaction between sulfur and water was found in the range of 500° to 700°C but not at lower temperatures. Terres et al [78] claimed that below 800°C , sulfur was the only product for such a reaction. Platinum and iron, both supported on clay, were used as catalysts. Doumani et al [25] carried out the same reaction over an iron-bauxite catalyst. The activity of the catalyst increased during the reaction, which was thought to depend upon greater activity of sulfides than of oxides. For bauxite catalyst, the reaction was found to start at 370°C and the rate became appreciable at 425° to 480°C . Gel type catalysts were also capable of starting the reaction below 325°C . Even at the lowest temperature studied, i.e. 316°C , a considerable amount of H_2S was found. Reaction between H_2O and S was also believed to occur.

2.3.4 Hydrogenation Reactions

The reduction of SO_2 by H_2 has been a reaction of interest for a long time [25, 39, 45, 69]. Berthelot [5] noted in 1898 that no homogeneous reaction occurred even at 280°C . At higher temperatures, H_2S was formed and at red heat, the reaction products were S and H_2O . Panchanon et al [62] found that nickel catalyzed the

formation of H_2S . It was believed that H_2S was formed partly by reduction of nickel sulfide and partly by reaction with sulfur dioxide enclosed in nickel sulfide. In contradiction to other workers, they found that precipitated nickel sulfide could be reduced by H_2 . Tomkinson [85] noticed that nickel caused incipient reaction at 280°C , but considerable reaction rate was obtained only above 350°C . The catalyst was gradually transformed to nickel sulfide, which was also an active catalyst above 300°C . Within the temperature range of 400° to 450°C , the reaction products were H_2O , H_2S and S . Other active catalysts for hydrogenation of SO_2 include cobalt sulfide and iron sulfide while copper and cadmium sulfides were inactive. In the absence of a catalyst, Tomkinson [85] could not detect any reaction even at 500°C . In the Carpenter and Evans process [11] CS_2 was decomposed by heat in the presence of hydrogen or coal gas according to the reaction,



Crawley and Griffith [22] studied the hydrogenation of COS between 125° and 200°C with nickel subsulfide as catalyst. From about 150°C upwards, the reaction was first order with respect to COS , but at lower temperature, some retardation occurred and the reaction approached zero

order. The cause of retardation was not clear but the authors suggested that it might be due to van der Waals adsorption of COS. Between 150° and 200°C, this type of adsorption would cease and the reaction then took place by collision of COS with adsorbed hydrogen. Bacon and Boe [4] found that the reaction between H₂ and S was fast above 350°C, giving a very pure H₂S.

2.3.5 Miscellaneous Reactions

The reduction of SO₂ with carbon has been thoroughly investigated by Imperial Chemical Industries [2] and Consolidated Mining and Smelting Co. of Canada [44, 45]. Reactions taking place in the coke bed were,

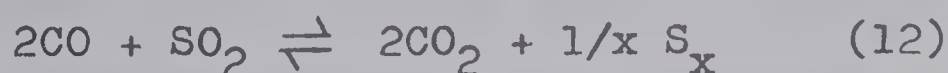
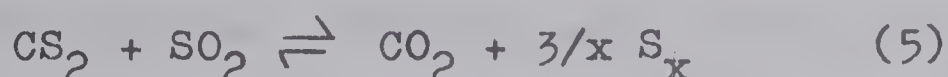
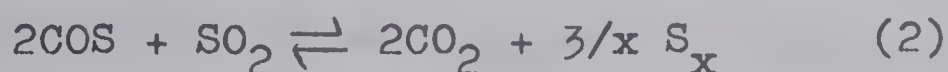
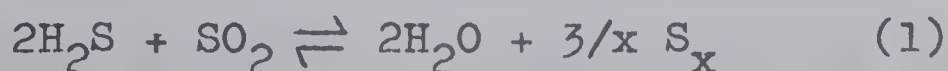


The reduction of SO₂ by C is strongly exothermic, whereas the reduction of CO₂ is endothermic. The rate of reaction between SO₂ and C was found to be faster than that of CO₂ [45]. When about 80 % of the SO₂ had been reduced, the temperature gradually increased to 1300°C. In order to carry the reaction to completion, two steps for the process were employed. First, a portion of the SO₂ was mixed with air and passed into the coke bed in an

apparatus similar to a gas producer. At the lower temperature, prevailing in the upper part of the bed, COS was formed as a result of the reaction of CO with S,



The gases left the producer at 700° to 900°C. Owing to this reaction, all the sulfur could be maintained in the gaseous phase so that the products of the first step of reduction could be carefully cleaned of dust before entering the second stage which consisted of reduction in the presence of a contact catalyst. Here, the remainder of SO₂ was mixed with the gases from the producer and the reactions which took place were,



H₂S and CS₂ were present as minor constituents in the reactants from the coke bed. The catalysts consisted of a sintered mixture of alumina and clay. The temperature in the catalyst bed was maintained between 250° and 500°C. After the reduction, the gases were passed through a waste

heat boiler in which separation of liquid sulfur began. The remainder was carried along as mist, which was finally separated in Cotrell precipitators.

It has been known that inorganic constituents, particularly iron in an easily reducible state, have a marked effect on the reactivity of coke [40]. Perrott [65] believed that without contaminants, the ultimate rate of combustion by SO_2 of any type of carbon with the same surface area would be the same. With domestic or other types of nonmetallurgical coke, high reactivity is due largely to the presence of hydrocarbons. Lepsoe [45] found that in the reduction of SO_2 with semicoke made from Michel coal containing 9% volatile hydrocarbons, rapid reaction occurred at 800°C -- a relatively low temperature. A copious quantity of H_2S was present in the reaction products. The reaction continued until 55% of the semicoke was consumed, when the coke became "inactive"; i.e. the remaining coke had acquired the characteristics of metallurgical coke and H_2S no longer appeared in the exit gas. With charcoal previously calcined at 1200°C , the reaction commenced at 650°C and continued at a fast rate at 800°C until 80% had been consumed. Yuskevitch [93] found that CH_4 and SO_2 reacted readily at 900°C in the presence of bauxite catalyst to form sulfur, H_2S and CO . The dry Thiogen Process, invented by Young [92] in 1912,

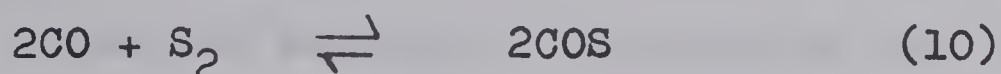
used hydrocarbons from cracking petroleum oils for producing sulfur direct from smelter gases. The catalyst was calcium sulfate which was assumed to undergo successive reduction to calcium sulfide with the hydrocarbons and reoxidation to calcium sulfate and sulfur with sulfur dioxide. The process was not commercially satisfactory because oxygen in the gases caused excessive losses of the hydrocarbon and also because, under the conditions used, the carbon was converted only to carbon monoxide. Bacon and Boe [4] studied the reaction between CH_4 and sulfur in the presence of water vapor at 300° to 650°C and obtained H_2S and CO_2 as product. Forney and Smith [27] and Nabor et al [56] measured the kinetics of the reaction between CH_4 and sulfur. The former authors found the rate equation to be

$$r = k P_{\text{CH}_4} P_{\text{S}_2}$$

at 600°C and 1 atm pressure, where $k = .26 \text{ gm mole CH}_4 / (\text{gm catalyst})(\text{hr})(\text{atm})^2$. The latter authors used silica as the catalyst at temperatures from 550° to 700°C , the rate equation was found to be the same as that obtained by the former authors. Their rate constant was expressed as,

$$\log k = 10.9 - 31,400/2.303RT$$

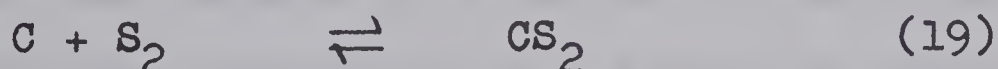
Partington et al [64], Stock et al [76] and Terres et al [79] studied the reaction between CO and S and showed that the reaction occurred in two consecutive steps,



over a temperature range of 300° to 550°C. The rate of decomposition of COS to CO and S was said to be very much faster than that of conversion to CS₂ and CO₂.

Madon et al [50] noted that the rate of reaction was high when CO was bubbled through liquid S at its boiling point containing a suspension of fine silica powder.

They also found the reaction



to be of fractional order with an activation energy of 13,000 cal/gm mole.

Carter [14] found that COS reacted with C to give CS₂. Terres et al [79] obtained H₂O and CS₂ as products from the reaction between H₂S and COS.

CHAPTER 3

THERMODYNAMIC ANALYSIS OF THE PROBABLE REACTIONS IN CLAUS PROCESS SULFUR PLANTS

3.1 Review of Methods for Calculating Thermodynamic Equilibria

The classical methods of calculating the distribution of products at thermodynamic equilibrium often involve the use of equilibrium constants. The best known probably are the NACA and Brinkley methods [6, 7, 8, 9]. However, these methods have certain complexities and difficulties with regard to initial guesses, generality, and convergence. Meissner et al [54] developed a so-called "reactor series method" to calculate the equilibrium composition of a system in which more than one reaction are taking place. The multiple reactions, homogeneous or heterogeneous, are reduced to a series of individual reactions occurring separately in a series of hypothetical reactors. This technique also involves the use of equilibrium constants. Equilibrium is attained when the compositions satisfy the equilibrium constants of all the reactions and also the material balance constraint.

Several techniques for determining the equilibrium composition in complex reaction systems have been reviewed by Zelenik and Gordon [99]. The free energy minimization method, suggested by White et al [91] in 1958,

eliminates the difficulties of classical methods and has since attracted much interest. Thermodynamic equilibrium is reached when the free energy has its minimum value. The free energy minimization method uses the steepest descent technique to minimize the free energy with the system subjected to material balance constraint. This method was extended by Kubert and Stephanou [43] to include not only gases but also condensed phases. Oliver et al [60] used a methane-water system to demonstrate the method in 1962.

3.2 Analysis of Thermodynamically Feasible Reactions in Claus Process Sulfur Plants

Reactions in the catalytic converters of Claus process sulfur plants are usually quite complex. When any one of these reactions is studied, it is also important to take into consideration the influence of other parallel reactions which may occur. Basically, thermodynamic limitations govern the feasibilities of such reactions hence, before further experiments are performed in the present studies, a preliminary investigation of the thermodynamically feasible reactions in Claus process sulfur plants is desirable. The free energy minimization method is used to calculate the equilibrium conversion and product distribution of 18 reactions believed to occur in Claus

sulfur plants. All of these reactions were under 1 atm pressure and at a temperature range of 300° to 1000°K, with a stoichiometric ratio of pure reactants and no products in the feed. A computer program called FREM was employed for the present equilibrium calculations. This computer program is listed in Appendix C .

A general equation of the form,



where a,b, etc. are stoichiometric coefficients was used to represent each reaction. Equilibrium conversion is defined as the conversion of reactant A under equilibrium conditions. The results obtained in the form of equilibrium conversions and product distributions at different temperatures for the 18 reactions are shown in tables C.3 to C.20 of Appendix C .

The equilibrium conversions of the following reactions which are expected to proceed beyond 50 % conversion are plotted as a function of temperature (from 300° to 1000°K) in figure 1 .

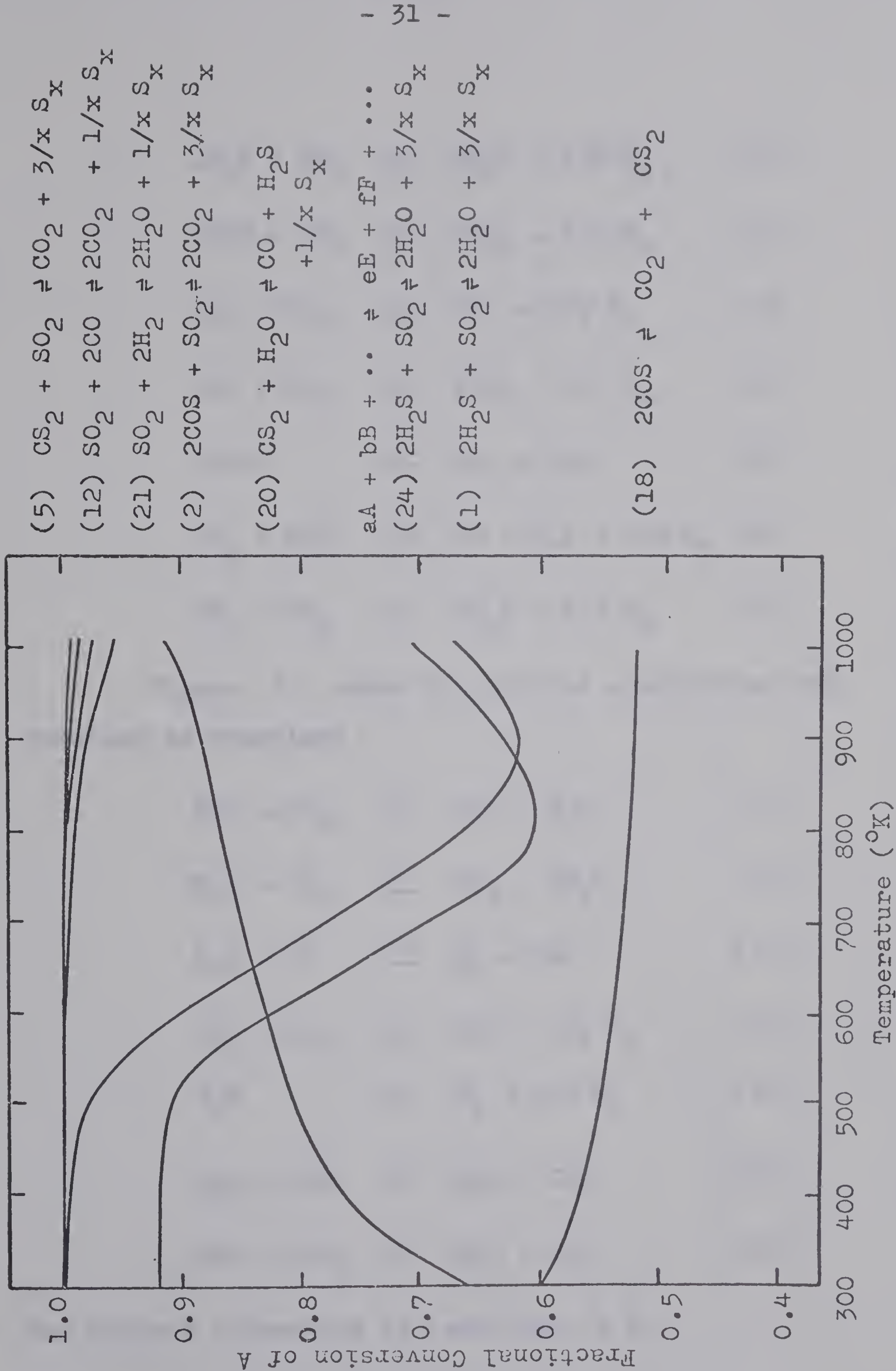


Figure 1 Equilibrium Conversion of the More Feasible Reactions

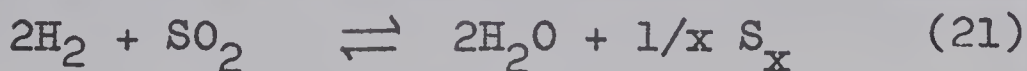
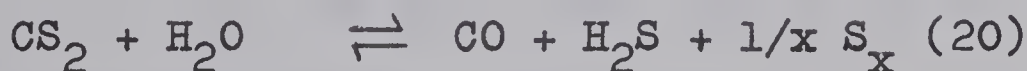
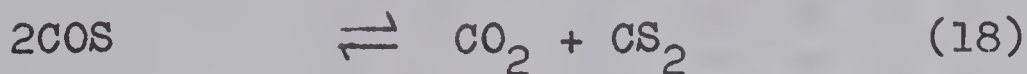
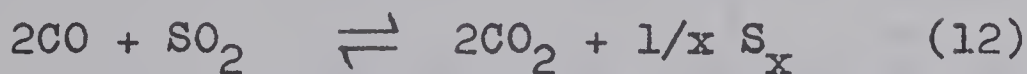
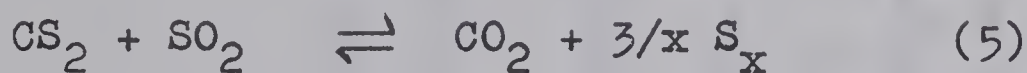
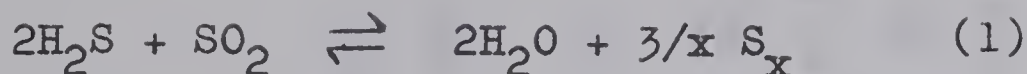
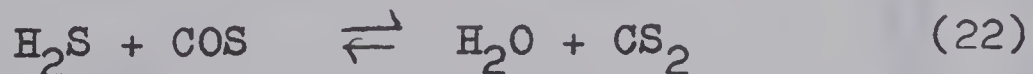
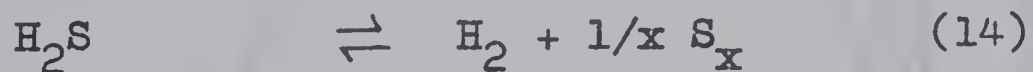
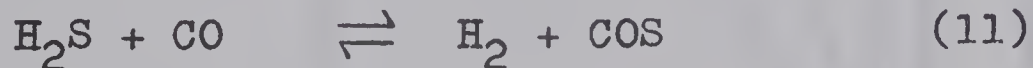
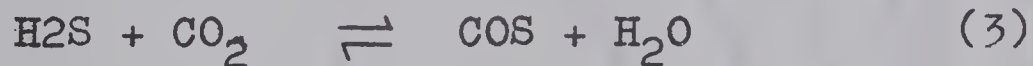


Figure 2 shows the plot of equilibrium conversions of reactions



The highest conversion is less than 25 %.

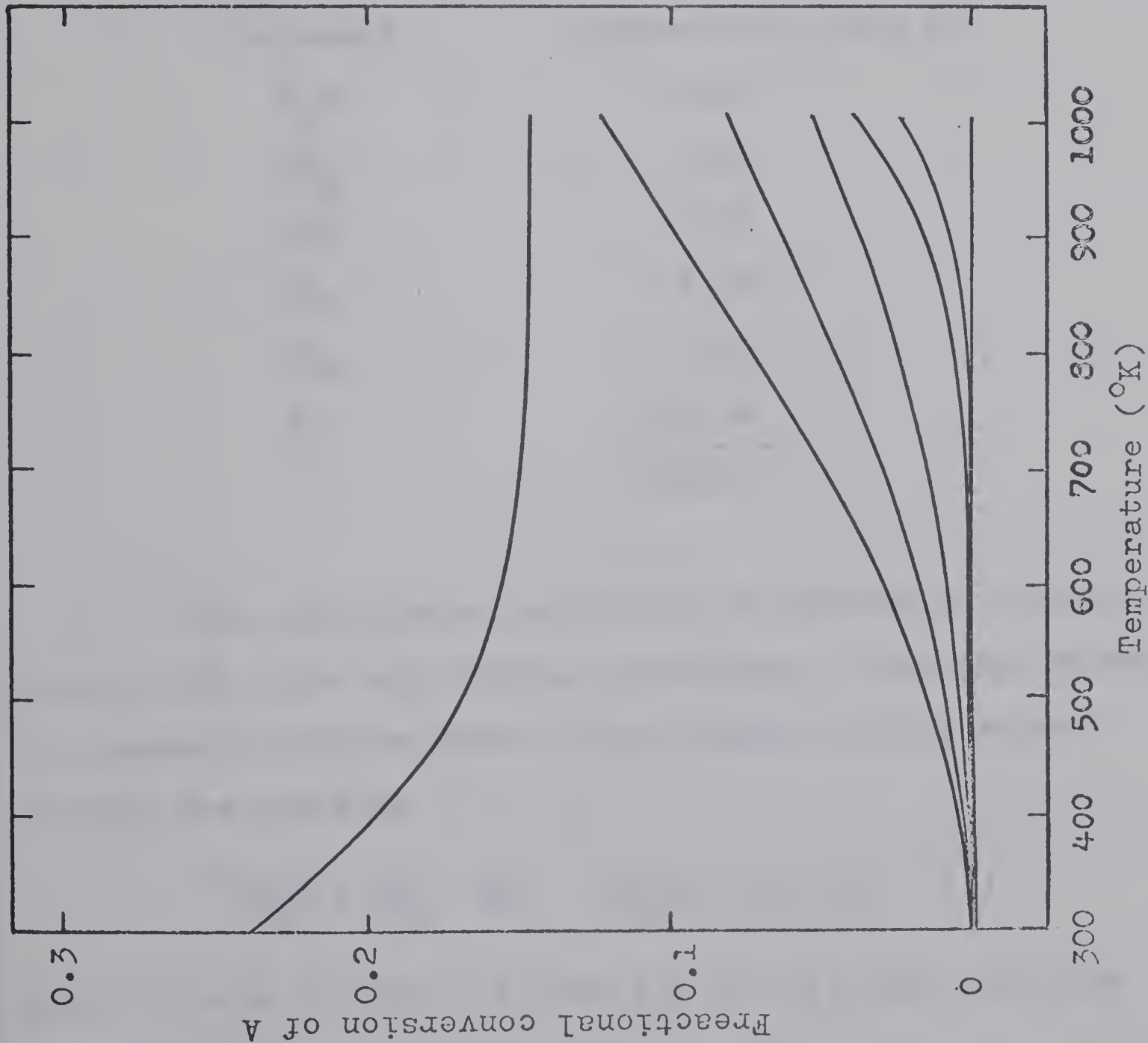


Figure 2 Equilibrium Conversion of Less Feasible Reactions



The first group of reactions exhibit predicted equilibrium conversions far higher than those of the second group and accordingly should be given more priority when considering the possible side reactions.

Curve (24) of figure 1 represents the plot of equilibrium conversion versus temperature of a typical feed from the waste heat boiler in an industrial plant with the following composition

Component	Composition (mole %)
H ₂ S	6.70
SO ₂	3.87
COS	0.95
CS ₂	0.32
CO ₂	7.70
N ₂	80.46
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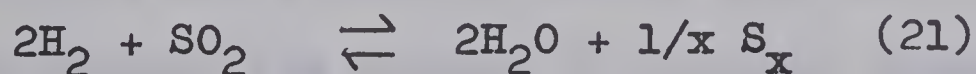
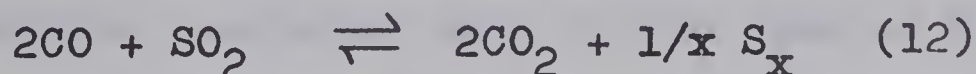
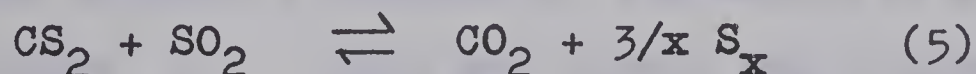
The equilibrium conversion is defined as conversion of H₂S under equilibrium conditions. When this curve is compared with the curve (1) of figure 1 which representing the reaction



with 2/3 mole fraction of pure H₂S and 1/3 mole fraction

of SO_2 in feed, it can be seen that at the same temperature, the equilibrium conversion for curve(24) is lower than that for curve (1) . This perhaps may be due to the competition for SO_2 by COS and CS_2 with H_2S .

From the results of thermodynamic analysis shown in figure 1 , it is apparent that at the reactor temperature of the industrial sulfur plants which is 500° to 550°K , the following reactions exhibit high equilibrium conversions



Reaction (1) is the major reaction in Claus sulfur plants. The concentrations of CO, H_2 and CS_2 are much lower than that of COS in the industrial reactors. Consequently the reactions which should be specifically considered in reactor design are reactions (1) and (2) . These are also reactions to be studied in the present work .

CHAPTER 4

EQUIPMENT AND EXPERIMENTAL PROCEDURE

The equipment was originally designed and built by McGregor [53]. A detailed description of the construction of the equipment had also been presented by him. Because a different experimental program was conducted in the present studies, some modifications to the equipment were required and these will be described later. The modified equipment can be utilized more flexibly in the future studies. The material of construction of the equipment was 316 stainless steel.

4.1 Flow and Metering System

The schematic diagram of the modified equipment is shown in figure 3 . Each gas bottle was equipped with its own pressure regulator and, in the case of nitrogen, a second regulator was placed in series with the first. This was done to improve the control of nitrogen pressure upstream of the flow controller. Each gas stream was dried with anhydrous calcium sulfate contained in 500 c.c. stainless steel cylinders before entering the system and silica gel was used for drying SO_2 because water catalyzed most of the Claus reactions. The dry gas streams were regulated by glass rotameters with stainless steel balls.

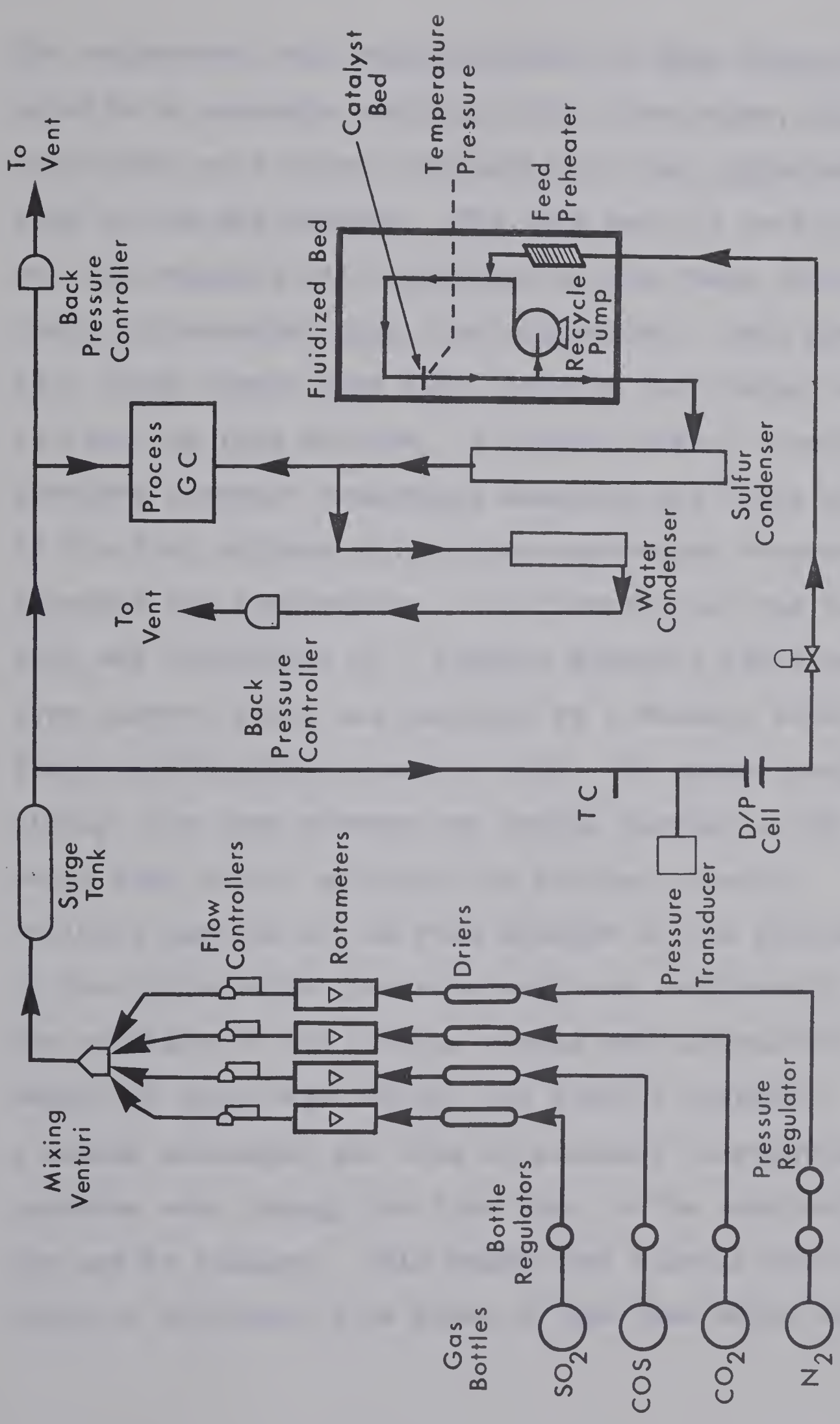


Figure 3 Schematic Flow Diagram of Modified Experimental Equipment

The rotameters were unsatisfactory in that they did not provide an accurate reading of the flow rates; they only functioned as a visual indication of the approximate flow-rate of the gas streams. The flow rate of each gas stream was set manually and controlled by the Moore 63BU-L constant differential type flow controller. Each gas stream, at a fixed steady flow rate, entered the mixing venturi to form the feed mixture. A Foxboro 66FR-2 electronic absolute pressure transducer measured the total pressure of the feed mixture and an iron-constantan thermocouple measured the temperature. The flow rate of the feed mixture was controlled by a Foxboro Stabiflo 6R-V4 needle type control valve and measured by a Foxboro 613DL electronic differential pressure cell. To ensure perfect mixing, the feed mixture was passed through a 500 c.c. surge tank before entering the reactor assembly. A variable portion of the feed mixture on the upstream side of the differential pressure cell was continuously vented. The quantity of the portion vented was determined by the amount of feed required for the reactor assembly. Such a design maintains the feed at constant composition and pressure even though its flow rate to the reactor assembly may be changed. This means that kinetic data can be taken at different flow rates of the feed while other

conditions remain unchanged. Another small portion of the feed was introduced continuously from the upstream side of the differential pressure cell to the gas chromatograph for analysis of the feed composition.

The recycle pump, recycle loop, and reactor were all immersed in the heated fluidized sand bath whose temperature was controlled at a fixed level. The feed stream was also preheated in the fluidized bath before entering the recycle loop. The recycle pump continuously circulated the gases through the catalyst in the reactor and around the recycle loop. The speed of the recycle pump was variable and thus the recycle rate of the gases could also be changed. The reliability of the recycle rate and the performance characteristics of the pump were described in detail by McGregor [53]. However, the recycle rate was fixed at a recycle ratio of 20:1 for the present work. An iron-constantan thermocouple imbedded in the center of the thin catalyst bed measured the reaction temperature and an Statham PA7327C absolute pressure transducer located at the side of the reactor bed, measured the reactor pressure. Sulfur was removed from the product stream in a condenser but water was still maintained as a superheated vapor. Condensed water was undesirable because it catalyzed the reaction. A portion of the

product stream exit from the sulfur condenser was introduced continuously into the gas chromatograph sampling valve for analysis of the product. The remaining portion flowed through a water condenser because water might catalyze the reaction between unconverted reactants in the vent line and sulfur, formed as product, might then plug up the vent line. A product back-pressure valve was used to control the flow of the final product stream to the vent. By regulating the split in product stream between the vent and the gas chromatograph and by adjusting the product back pressure valve, the reactor pressure could be varied.

4.2 Feed and Product Analysis

Both feed and product streams were analyzed by a Beckman-320 process gas chromatograph.

A number of ways to separate N_2 , CO_2 , COS , H_2S , CS_2 and SO_2 are described in the literature. Obermiller [59] used a novel dual column with Poropak Q packing to separate air, H_2S , SO_2 and A. Anon [1] performed the same separation with two different columns: the first was a 4 foot column packed with 15 % Ucon on 40/60 mesh Teflon T-6 and the second was a composite column of 5 feet of Chromosorb P followed by 7 feet of

molecular sieve 13X. Freeport Sulfur Co. [28] used silica gel packing to separate air, CO_2 , COS, H_2S , CS_2 and SO_2 . A dual column arrangement was employed for the present studies which involved the analysis of three types of gas mixtures with different constituents. The following sections describe the gas chromatograph operations for separating different types of gas mixtures.

4.2.1 Separation of N_2 , H_2S , SO_2 and H_2O

Two columns were used for this separation. The first column was a 7 foot long $\frac{1}{4}$ inch diameter stainless steel tubing packed with 25 % by weight of polyethylene glycol 15/200 on 30/42 mesh Teflon T-6 (HP) and the second column was 8 inch long $\frac{1}{4}$ inch diameter stainless steel tubing packed with silica gel.

A schematic flow diagram of the gases in this separation is shown in figure 4 . The stream selector valve shown in figure 5 enabled the selection of either feed or product streams for analysis. Referring to figure 4 , during feed analysis (shown as $\text{---}\cdot\text{---}\rightarrow$ flow) the feed stream passed through to the sampling valve

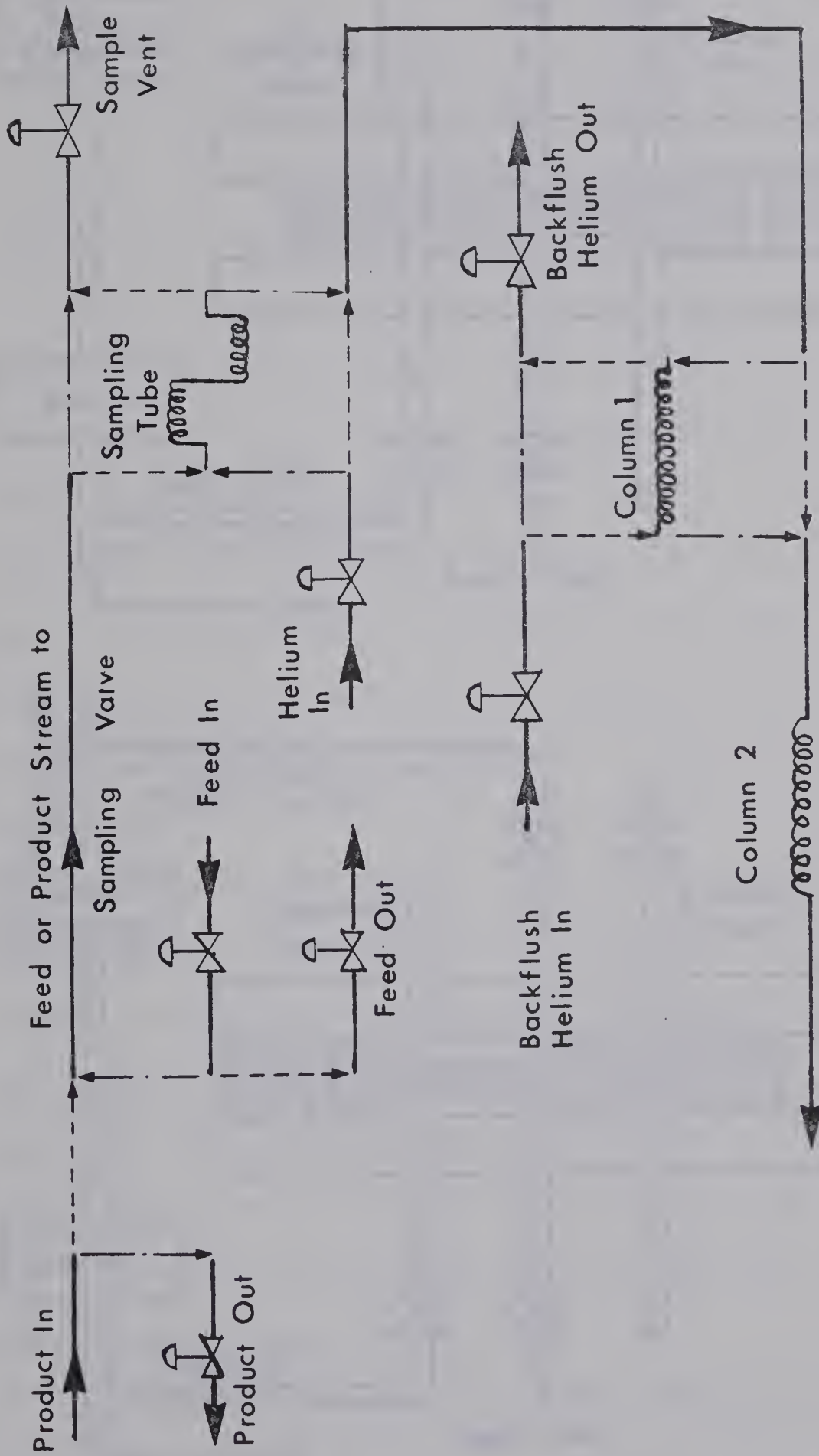


Figure 4 GC Flow Diagram for Separation of N_2 , H_2O , H_2S and SO_2

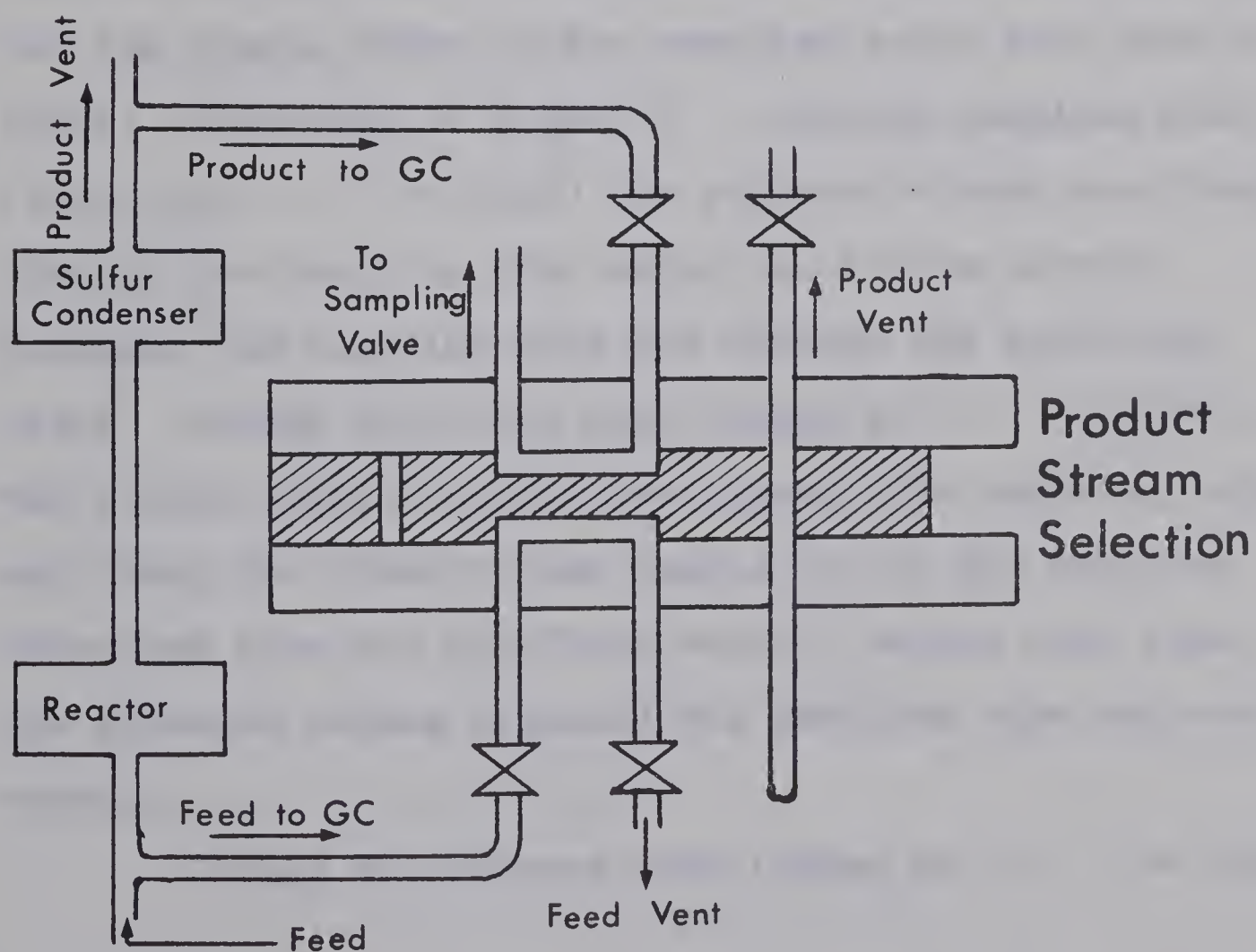
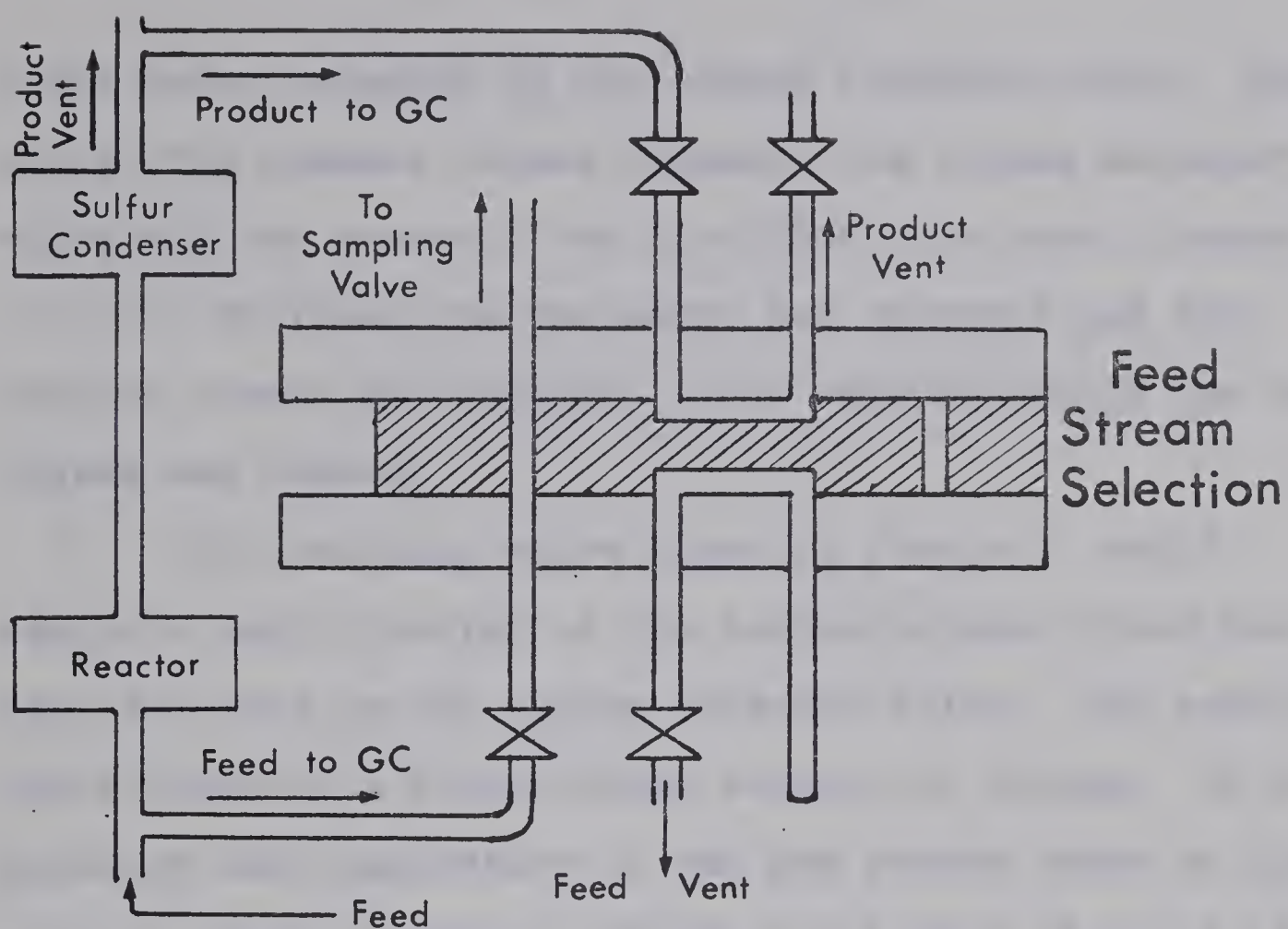






Figure 5 Stream Selector Valve

after being selected by the stream selector valve. Meanwhile, the product stream bypassed the stream selector valve and was vented. For the other flow mode, (shown as  flow) the procedure was reversed and the product stream was selected to be analyzed while the feed stream was vented.

The sampling valve shown in figure 6 would sample a small portion of the desired stream which had been selected by the stream selector valve. The sampling valve contains a fixed-volume section of tubing. If the pressure and temperature of the gas stream taken by the stream selector valve is fixed, the number of moles of the gas sample taken by the sampling valve will also be fixed. Referring to figure 4, during sampling mode (shown as  flow) the selected stream was flowing through the sampling tube while the helium carrier bypassed the sampling tube and entered the backflush valve. During the other mode (shown as  flow), the helium carrier would flow through the sampling tube and flush the fixed-volume sample out of the sampling valve and into the backflush valve. During this time, the selected stream bypassed the sampling tube and was vented.

During the forward mode (shown as  flow)

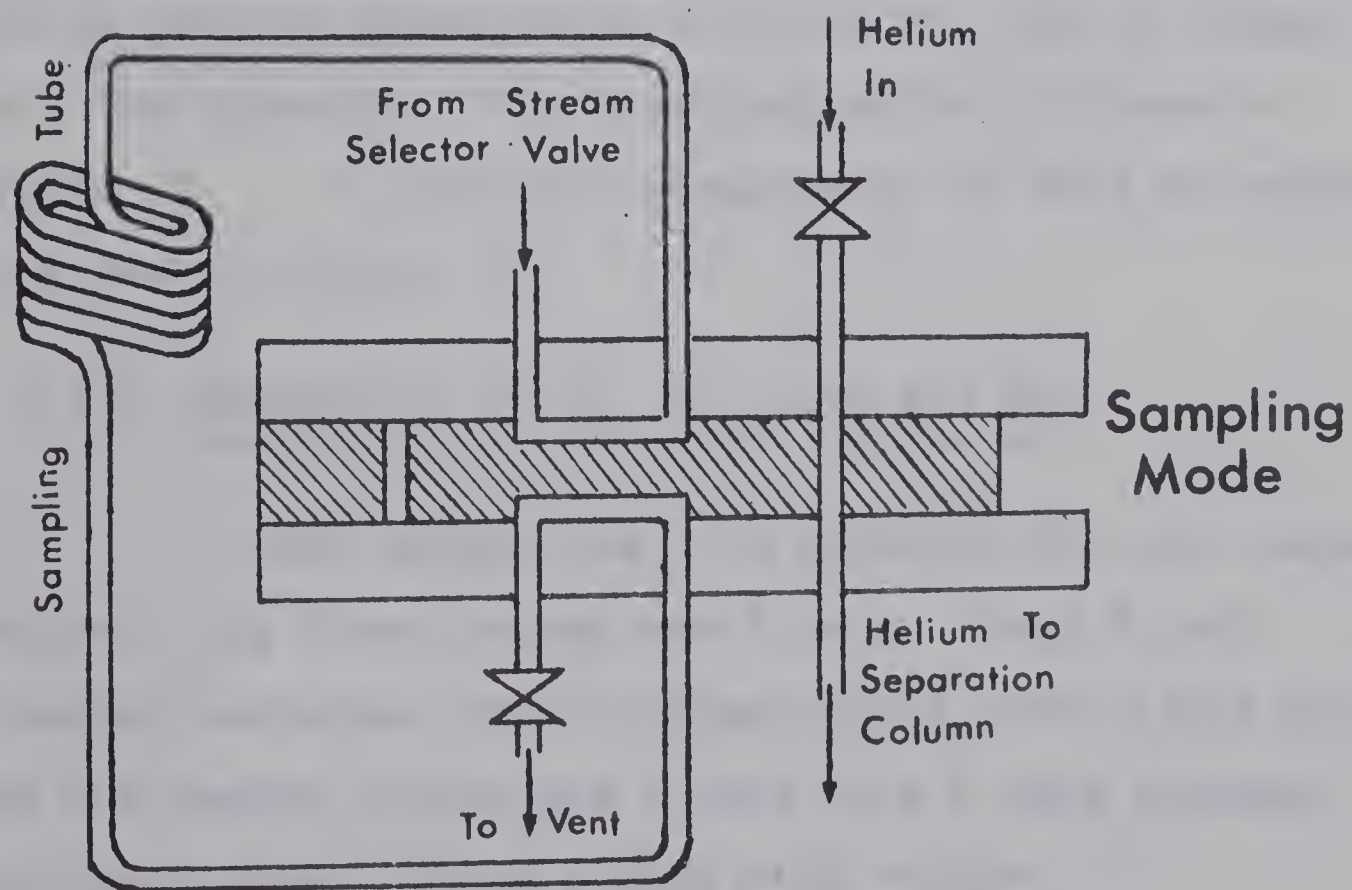
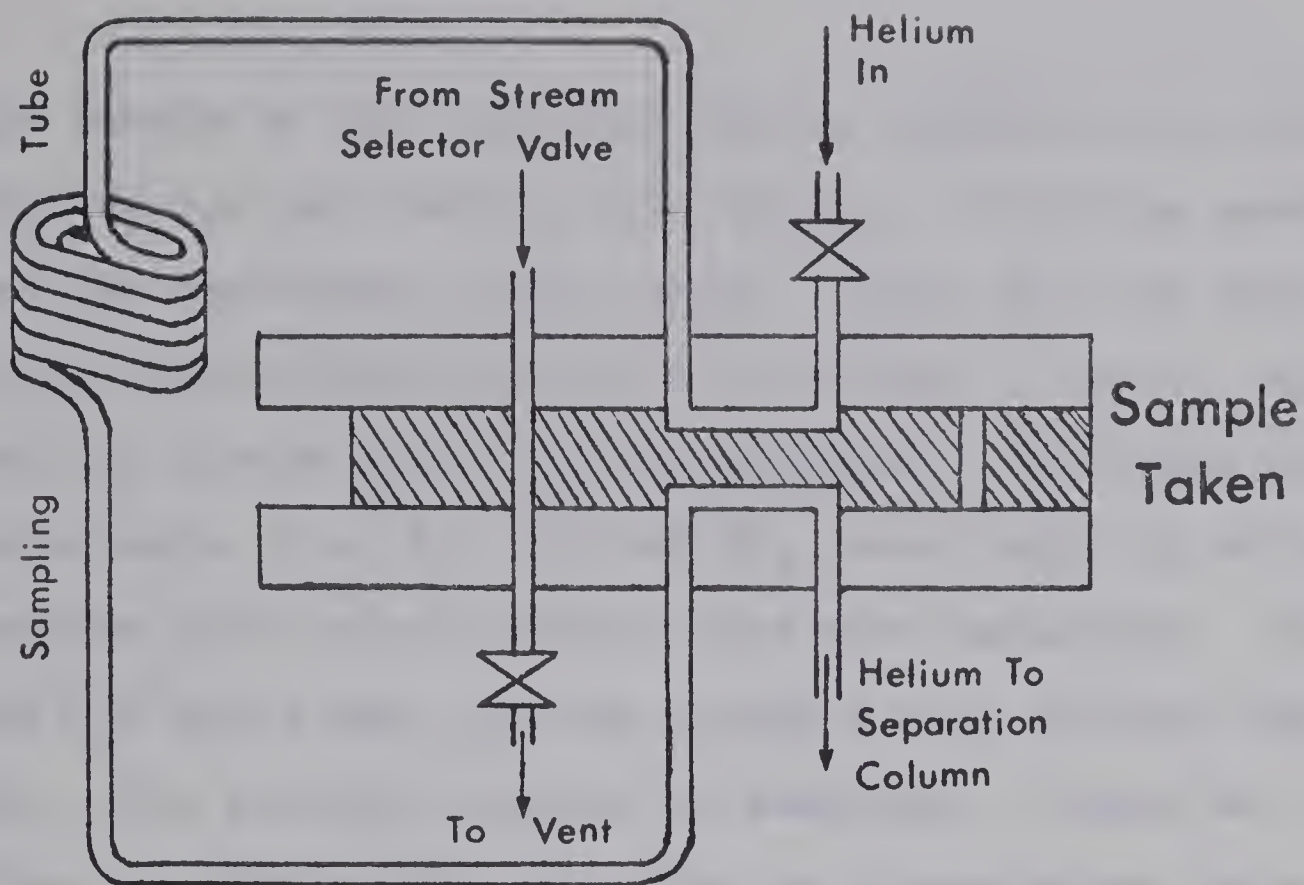


Figure 6 Sampling Valve

the sample in the backflush valve, containing N_2 , H_2S , SO_2 and H_2O was carried into column 1 by helium carrier and the backflush helium vented. Since H_2O was relatively more tenaciously held by column 1, the N_2 , H_2S and SO_2 eluted while H_2O was retained. The three eluted components, i.e. N_2 , H_2S and SO_2 , were swept by helium carrier into column 2 where they were separated. The N_2 and H_2S would pass through column 2 much earlier than SO_2 . The mode was changed to backflush (shown as --- \rightarrow flow) as soon as the complete gas chromatogram peaks of N_2 and H_2S were found. During this mode, helium would backflush the retained H_2O out of column 1 to vent while helium carrier transferred uneluted SO_2 out of column 2 into the detector. The backflush valve is shown in figure 7 . A complete chromatogram of such an analysis is shown in figure 8 .

4.2.2 Separation of N_2 , CO_2 , COS and SO_2

A dual column was also employed for this separation. The first column was 8 inch long $\frac{1}{4}$ inch diameter stainless steel tubing packed with silica gel and the second column was 2 foot long $\frac{1}{4}$ inch diameter stainless steel tubing packed with silica

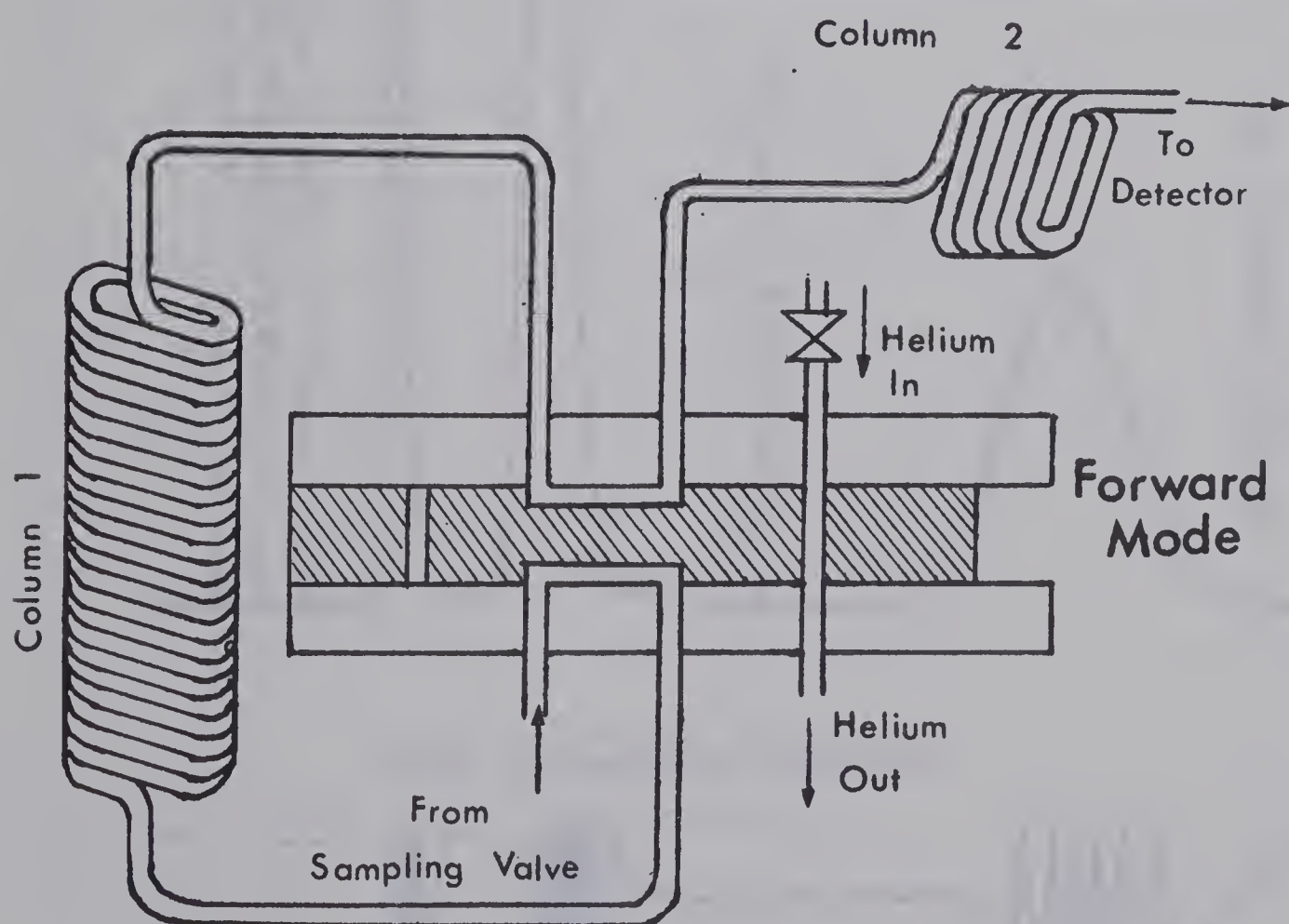
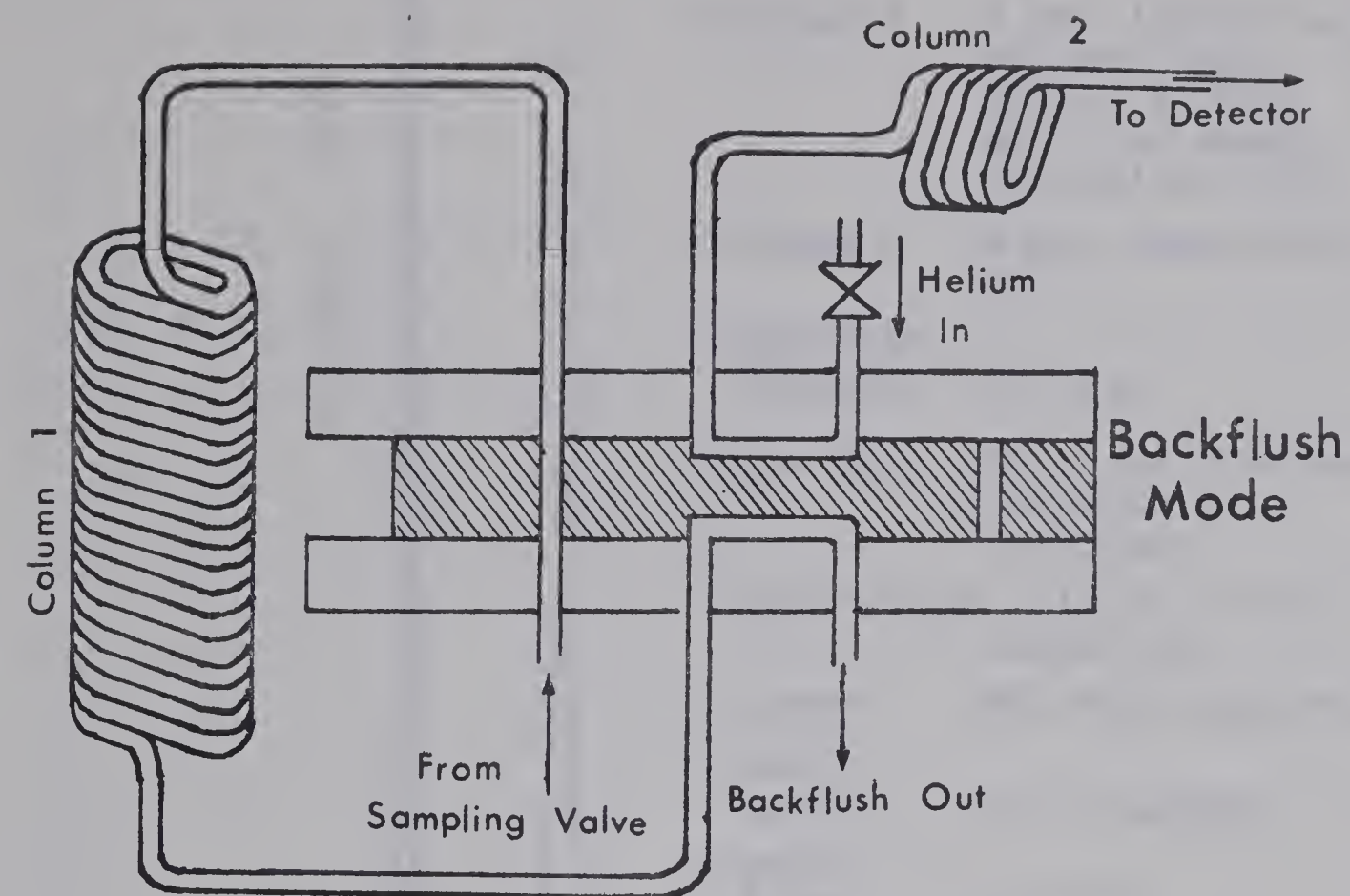
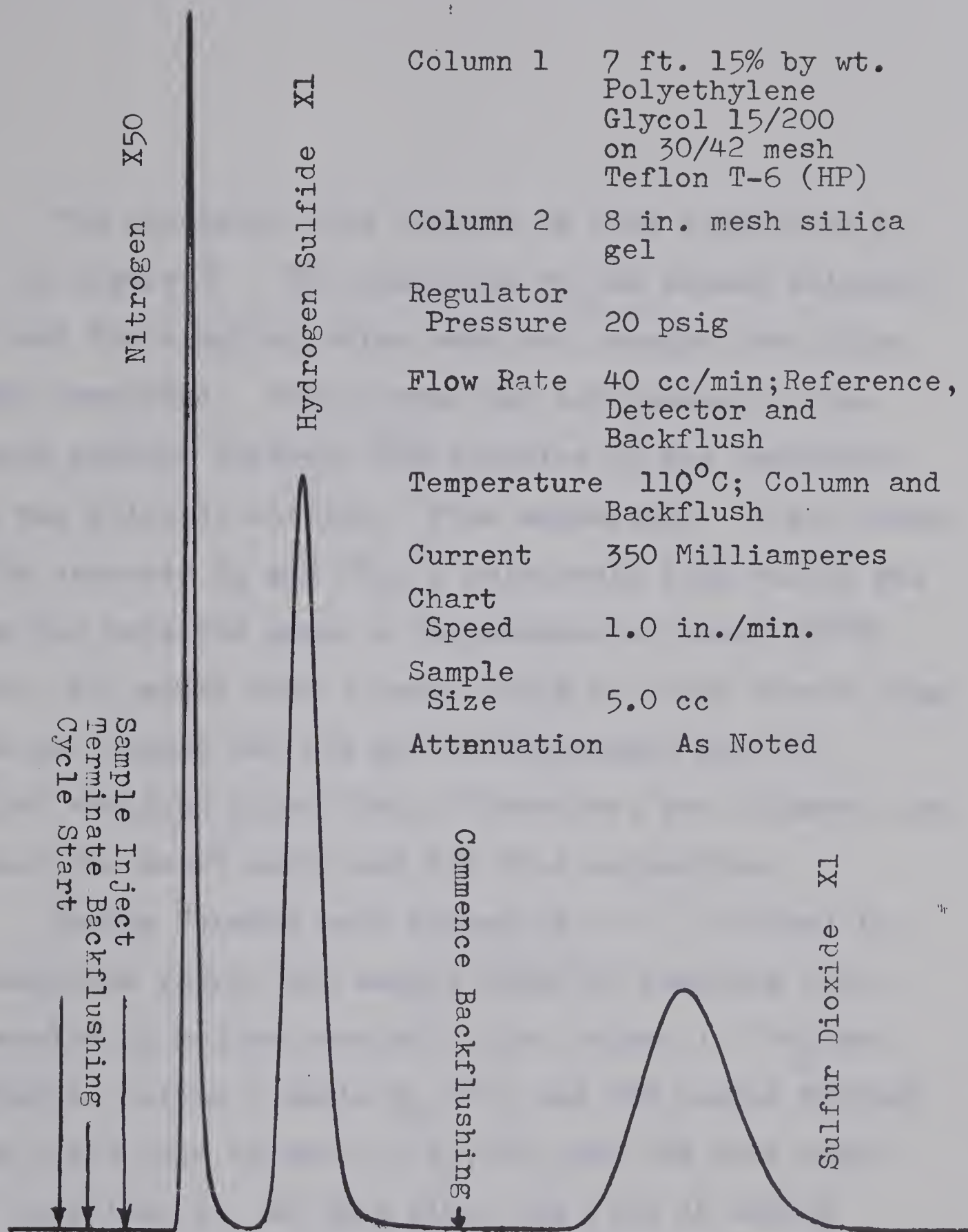


Figure 7 Backflush Valve



Column 1 7 ft. 15% by wt.
Polyethylene
Glycol 15/200
on 30/42 mesh
Teflon T-6 (HP)

Column 2 8 in. mesh silica
gel

Regulator
Pressure 20 psig

Flow Rate 40 cc/min; Reference,
Detector and
Backflush

Temperature 110°C; Column and
Backflush

Current 350 Milliamperes

Chart
Speed 1.0 in./min.

Sample
Size 5.0 cc

Attenuation As Noted

Disk Integrator Results

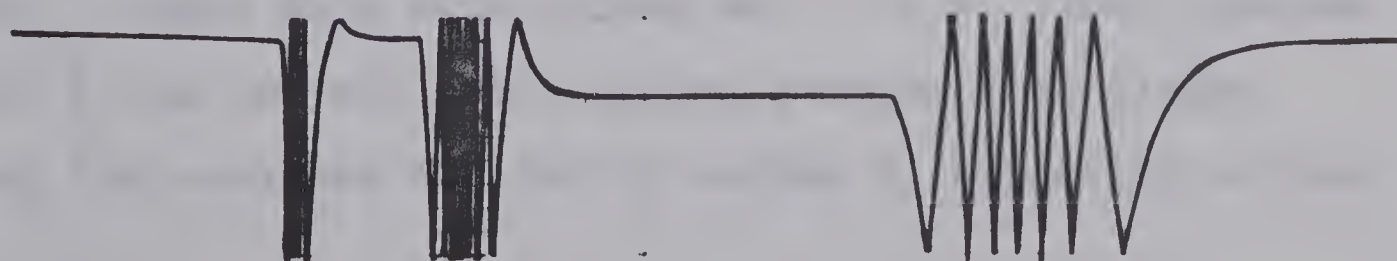


Figure 8

Typical Chromatogram for Separation of N_2 , H_2S and SO_2

gel.

The schematic flow diagram of this separation is shown in figure 9 . The functions of the stream selector valve and the sampling valve were not changed from those already described. Since water was not present in the feed and product streams, the function of the backflush valve was slightly altered. From experience, it was noted that to separate N_2 and CO_2 , a relatively long silica gel column was required under a temperature of about $210^{\circ}F$. However, SO_2 would take a long period to elute from a long silica gel column and the gas chromatograph peak so obtained would be quite flat. Therefore, two columns, one long and one short were used for this separation.

During forward mode (shown as $\text{---} \cdot \rightarrow$ flow) in the backflush valve, the sample taken by sampling valve was carried by helium carrier 1 into column 1. SO_2 was retained in column 1 while N_2 , CO_2 and COS passed through column 1 and into column 2. N_2 , CO_2 and COS were separated in column 2. At this time, the flow of helium carrier 2 was cut out. When the complete gas chromatogram peaks of N_2 , CO_2 and COS were obtained, the flow mode was changed. Hence this time (shown as $\text{----} \rightarrow$ flow), helium carrier 1 was cut off while helium carrier 2 continued pushing the retained SO_2 out of column 2, bypassing column

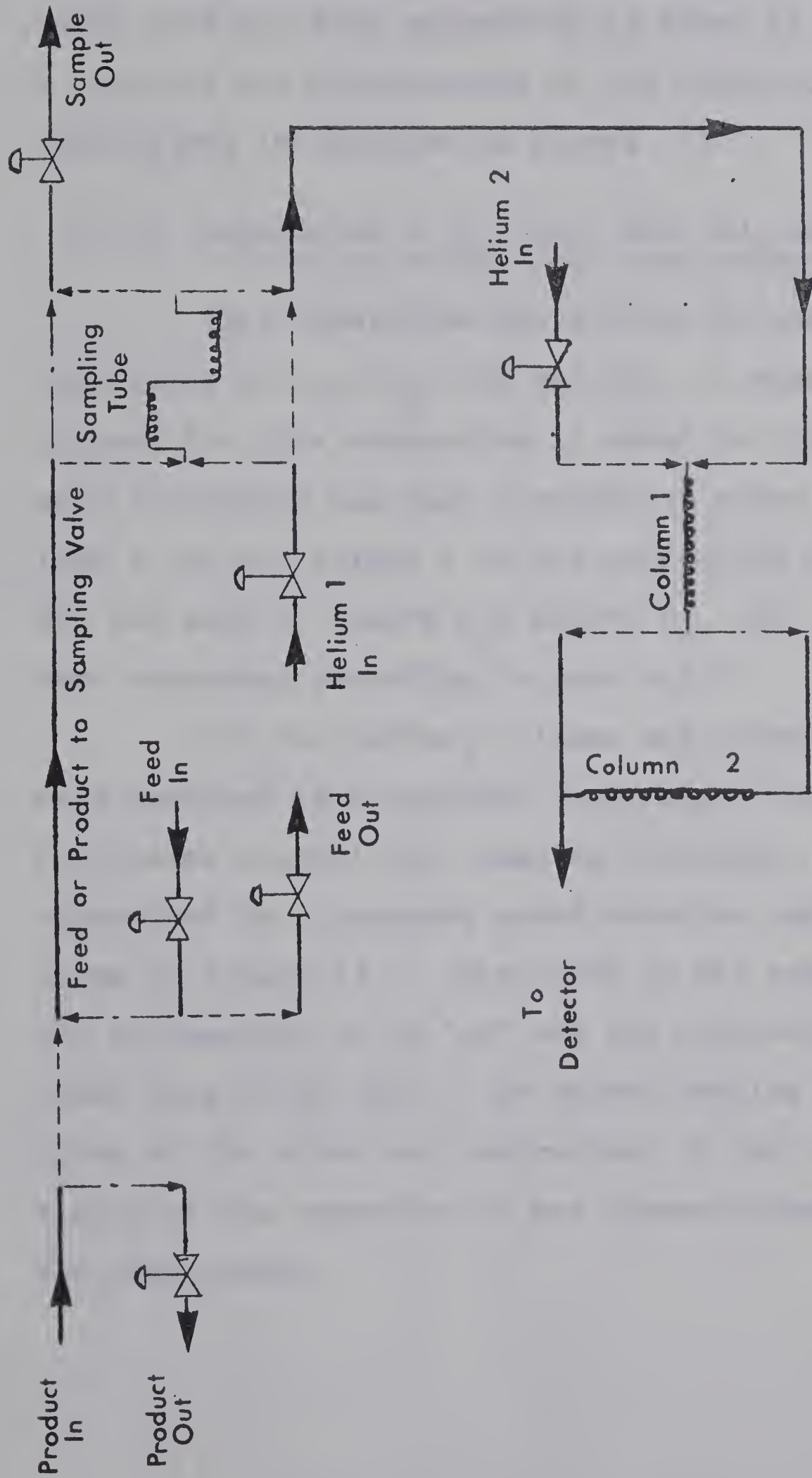


Figure 9 GC Flow Diagram for Separation of N_2 , CO_2 , COS and SO_2

2 into the detector. The configuration of the backflush valve used for this separation is shown in figure 10 . A complete gas chromatohram of the separation of N_2 , CO_2 , COS and SO_2 is depicted in figure 11 .

4.2.3 Separation of N_2 , CO_2 , COS, SO_2 and H_2O

This separation was similar to that used in the separation of N_2 , CO_2 , COS and SO_2 . A schematic flow diagram for this separation is shown in figure 12 . The only difference was that a backflush valve containing column 1 but not column 2 of the separation of N_2 , H_2S and SO_2 was used to remove H_2O before N_2 , CO_2 , COS and SO_2 were separated according to part 4.2.2.

All the valves, columns and connection lines were immersed in a constant temperature compartment. The timing control for changing flow mode, etc., was supervised by a constant speed rotation cam drive as shown in figure 13 . The slots in the cams would cause the microswitch to be "on" and the protrusions would cause them to be "off". By proper setting of the positions of the slots and protrusions of the cams, the timing of the operation of gas chromatograph analysis was thus preset.

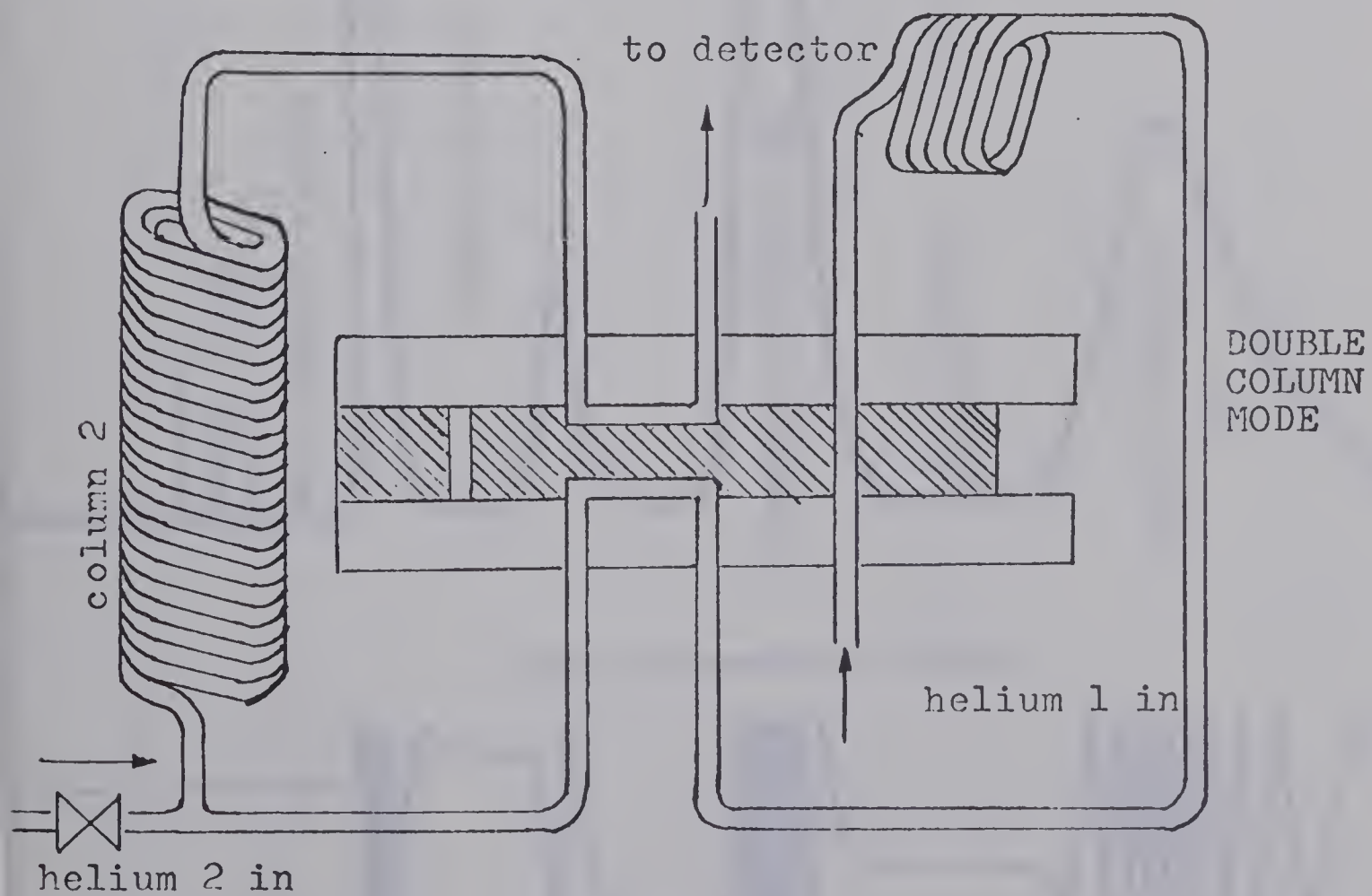
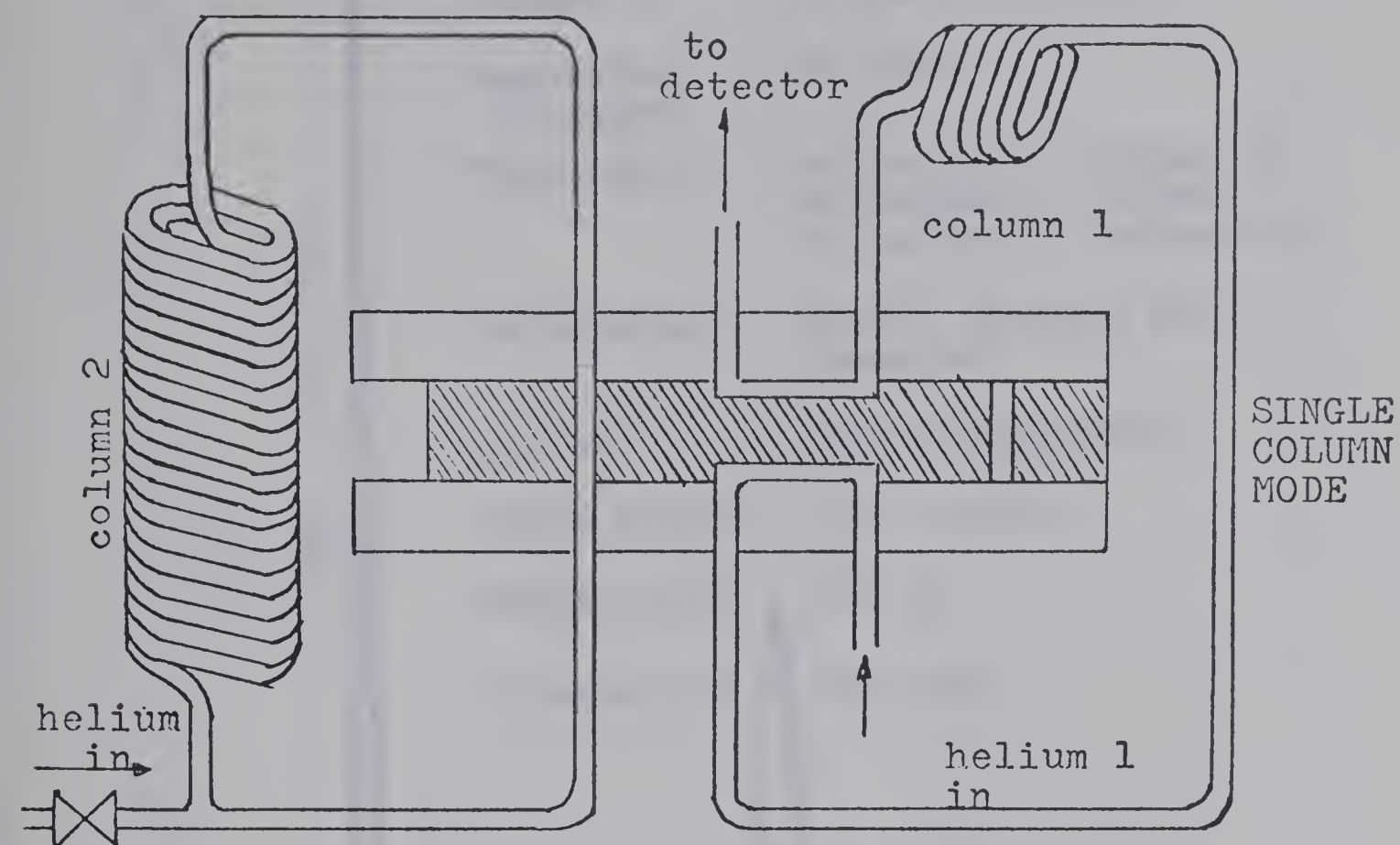
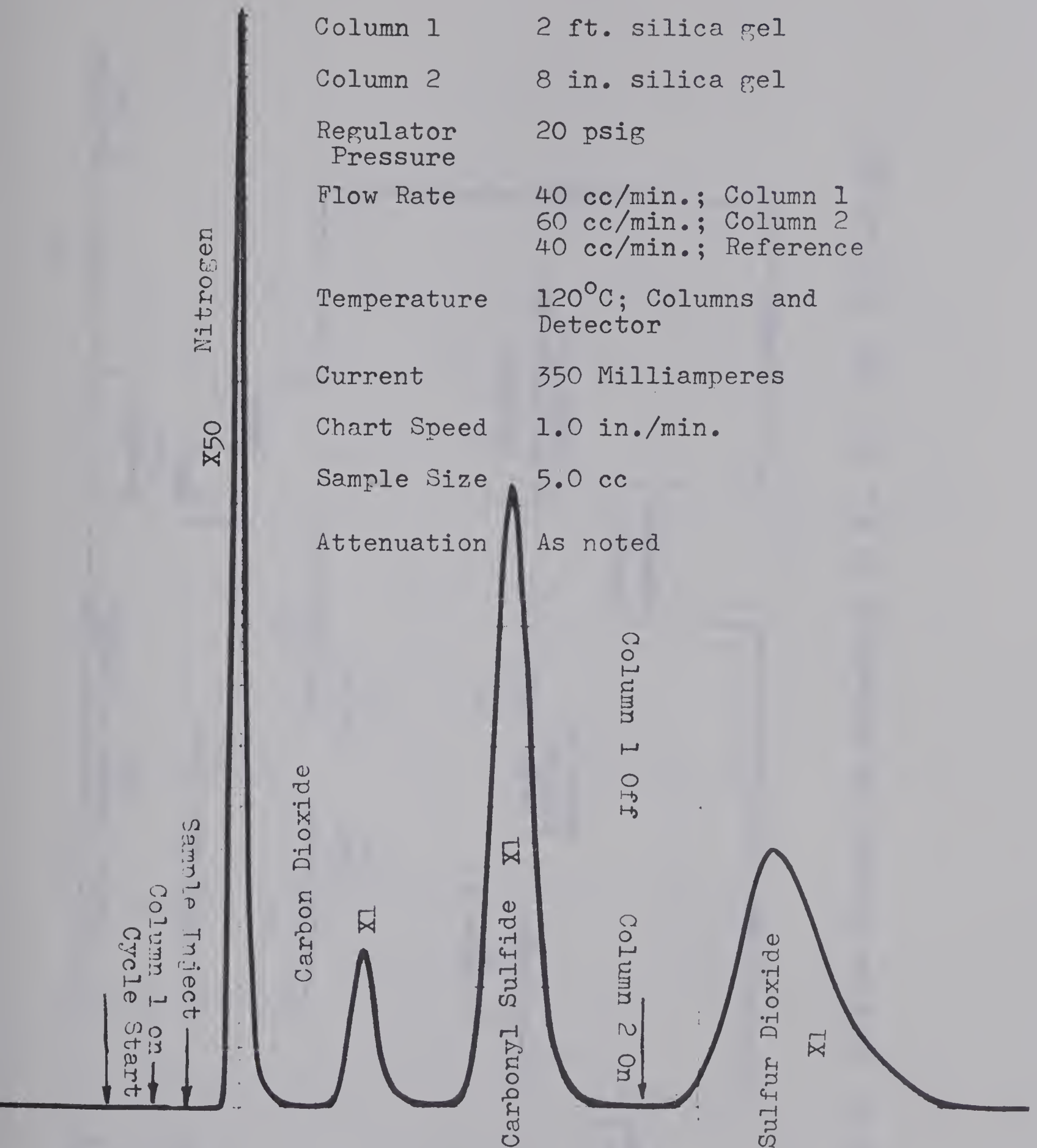


Figure 10 Column Switching Valve



Column 1	2 ft. silica gel
Column 2	8 in. silica gel
Regulator Pressure	20 psig
Flow Rate	40 cc/min.; Column 1 60 cc/min.; Column 2 40 cc/min.; Reference
Temperature	120°C; Columns and Detector
Current	350 Milliamperes
Chart Speed	1.0 in./min.
Sample Size	5.0 cc
Attenuation	As noted

Disk Integrator Results



Figure 11 Typical Chromatogram for Separation of N_2 , CO_2 , COS and SO_2

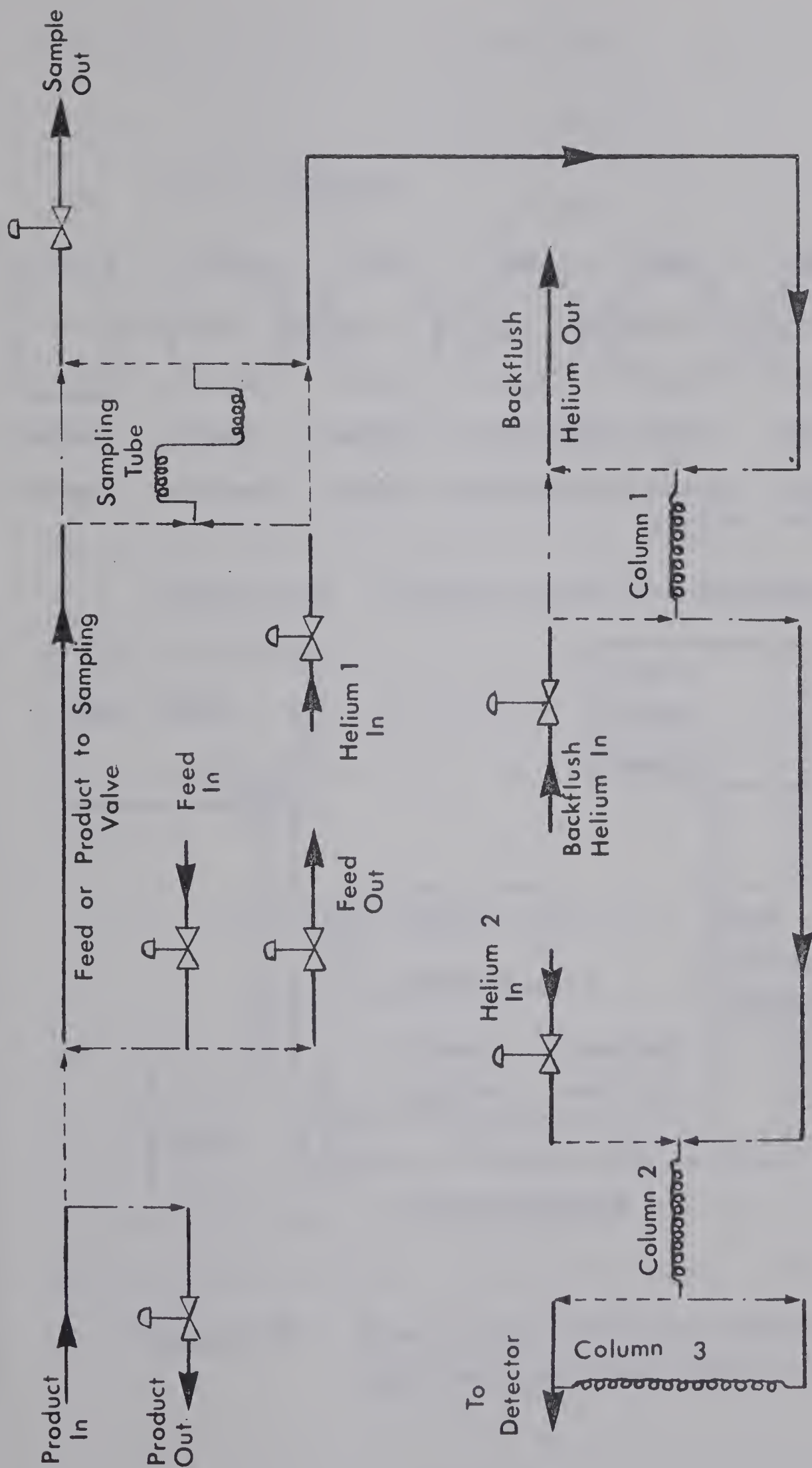


Figure 12 GC Flow Diagram for Separation of N_2 , CO_2 , COS , SO_2 and H_2O

micro switches

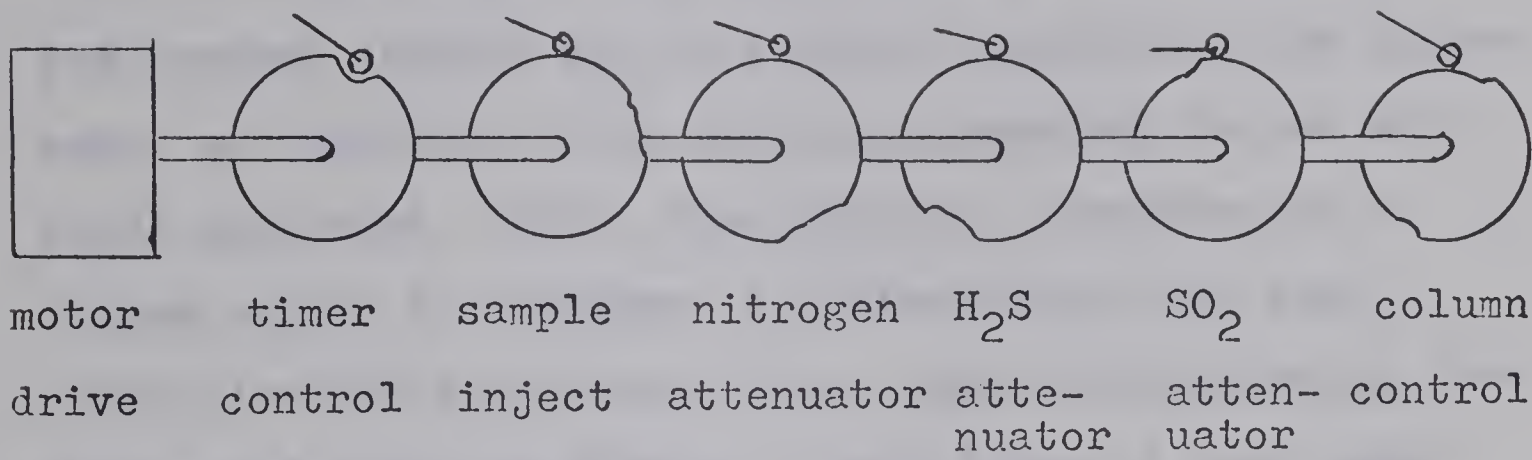


Figure 13A Typical Timer Cam Settings

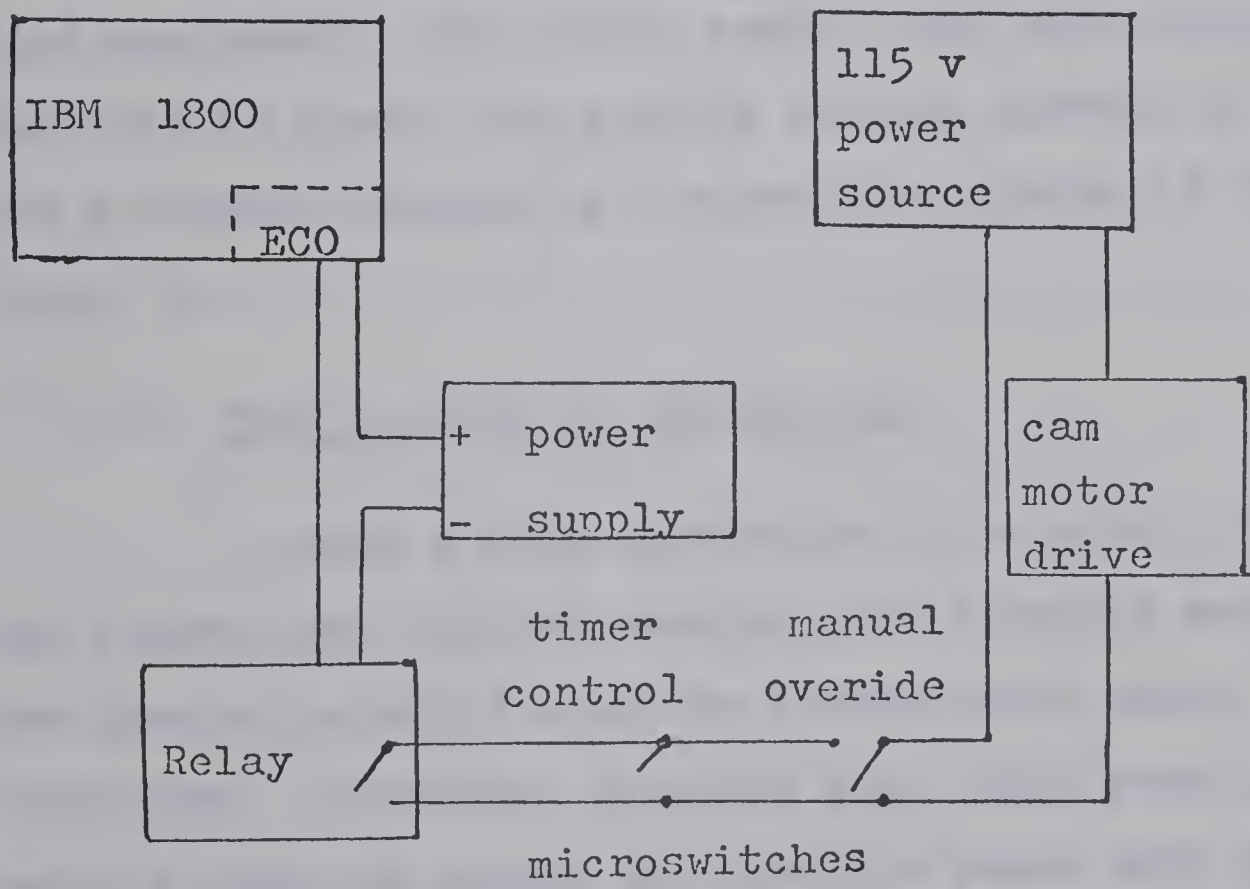


Figure 13B Electrical Interface Between ECO
And Programmer Cam Motor Drive

4.3 Modification of the Equipment

4.3.1 Addition of Another Gas Feed

To enable the equipment to be applicable to the present studies and to provide flexibility for future uses, an additional feed line was connected to the original equipment [53]. The addition, consisted of a drying agent, a rotameter, a differential type flow controller and connecting lines, duplicated existing feed source and metering devices. Four types of feed gases (instead of three) can now be introduced using the modified equipment. The mixing venturi was also slightly modified to blend four gaseous streams instead of three. The schematic diagram of the modified system is shown in figure 3.

4.3.2 Modification of the Reactor

Where a high conversion is required, the original reactor was limited because only slightly more than one gram of catalyst could be charged even under overload conditions. Moreover, catalyst dust could pass into the recycle pump and damage the graphite vanes when the reactor was disconnected from the recycle loop. The reactor

system was modified to eliminate these inconveniences.

The reactor assembly as well as part of the recycle loop shown in figure 14 were fabricated from stainless steel 316. The direction of flow of gases through the reactor assembly was from top to bottom (as shown in figure 14). The clearance between the walls of the reactor and the fluidized sand bath compartment of the original equipment was too small to allow for a larger reactor. To overcome this, the manifold which connected the exit of the reactor to the recycle pump was redesigned as shown in figure 14 . The increased space thus provided permitted a reactor with diameter as large as $1\frac{3}{4}$ inch to be used compared to the original $1\frac{1}{2}$ inch diameter reactor. Moreover, it was possible to interchange reactors of different sizes with the redesigned manifold.

The modified reactor differed in shape from the original one, being narrow at both ends and wider in the middle. Such a shape was necessary because the two ends of the reactor were connected to swagelock fittings of fixed size, $1\frac{1}{2}$ inch diameter. As a result, when the reactor was enlarged it was desirable to use the same swagelock connections. The total depth of the modified reactor was $\frac{3}{4}$ inch and catalysts could be charged to a

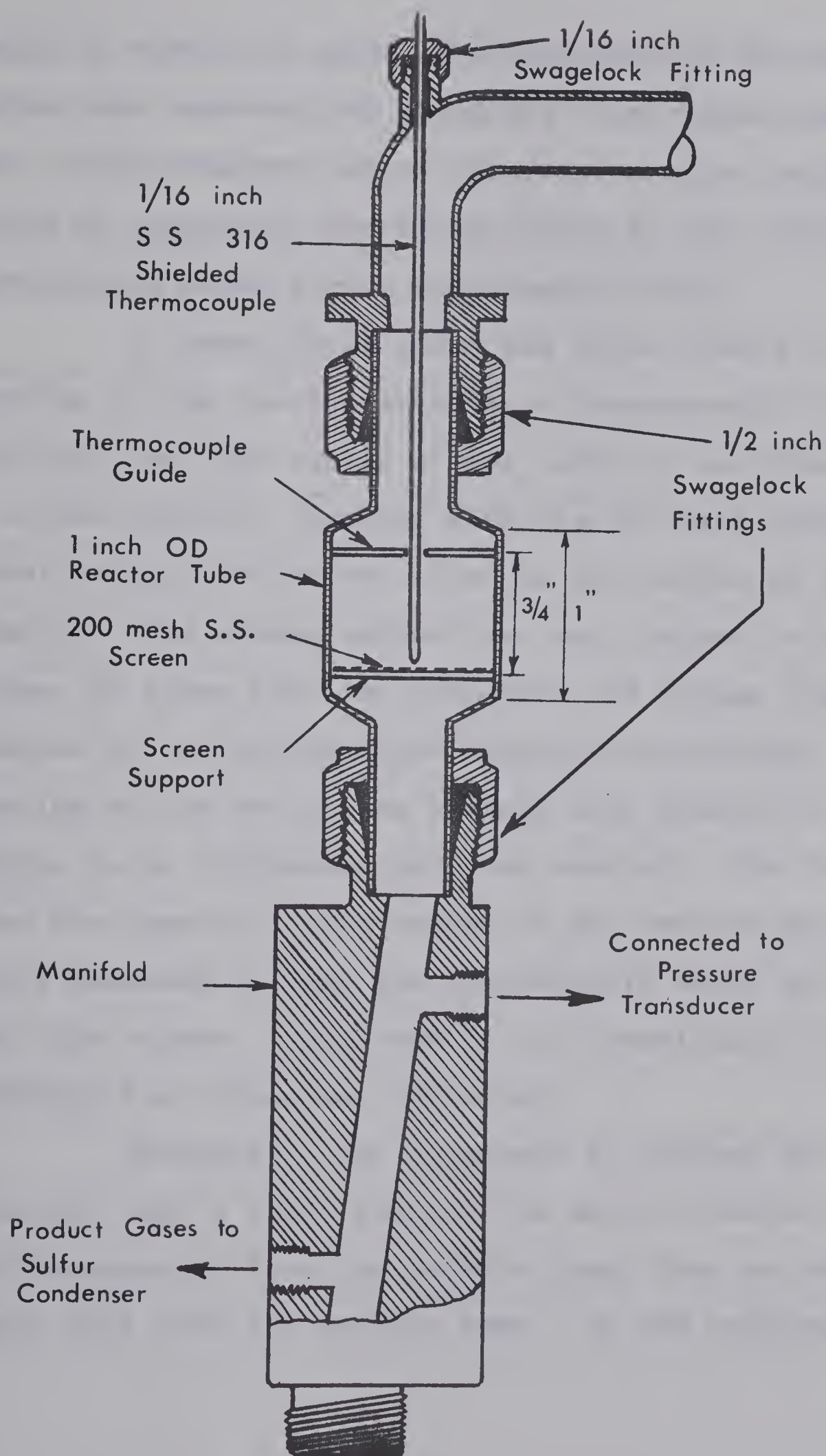


Figure 14 Modified Reactor

depth of about 1/2 inch. The remainder of the reactor volume was reserved for stainless steel balls placed on top of the catalyst bed so that the catalyst particles could be prevented from being eluted by the turbulence of circulating gases during experimental runs.

A thermocouple guide was press-fitted to the top portion of the reactor enabling a thermocouple to be introduced into the center of the catalyst bed from the top. A screen support, together with the 200 mesh stainless steel screen were press-fitted to the bottom of the reactor. The screen support not only helped to keep the screen in place but also protected the screen from being pierced by the thermocouple through carelessness. An opening on the top of the recycle loop enabled a thermocouple to be introduced into the reactor. The distance from the opening to the screen of the reactor was carefully measured so that the thermocouple would not contact the screen. Consequently, the possibility of breaking the screen was minimized.

Whenever it was necessary to replace the used catalyst with a fresh charge, The entire reactor could be disconnected from the recycle loop, thus no catalyst would fall into the recycle pump. In the original

reactor, the thermocouple entered the reactor from the bottom and after removal of this thermocouple, a hole in the catalyst support remained.

4.3.3 Modification of the Sulfur and Water Condensers

The complete product stream from the reactor, carrying sulfur vapor and other constituents, entered the sulfur condenser. The holdup capacity of the original horizontal sulfur condenser [53] was inadequate. To ensure a more complete removal of sulfur and to allow for the accumulation of larger amounts of condensed sulfur to permit more extended periods of operation, it was necessary to redesign and construct the sulfur condenser. Similarly, the water condenser should also be expected to meet such requirements. The modified water and sulfur condensers are shown in figure 15.

The lines from the reactor to the sulfur condenser, from the sulfur condenser to the gas chromatograph, and from the sulfur condenser to the water condenser were well-heated by wrapping with a nichrome wire heater so that sulfur vapor was prevented from condensing. Any condensation of sulfur in the lines would lead to a reduction in gas flow rate and eventual blockage of the line. The sulfur condenser was also heated with nichrome wire

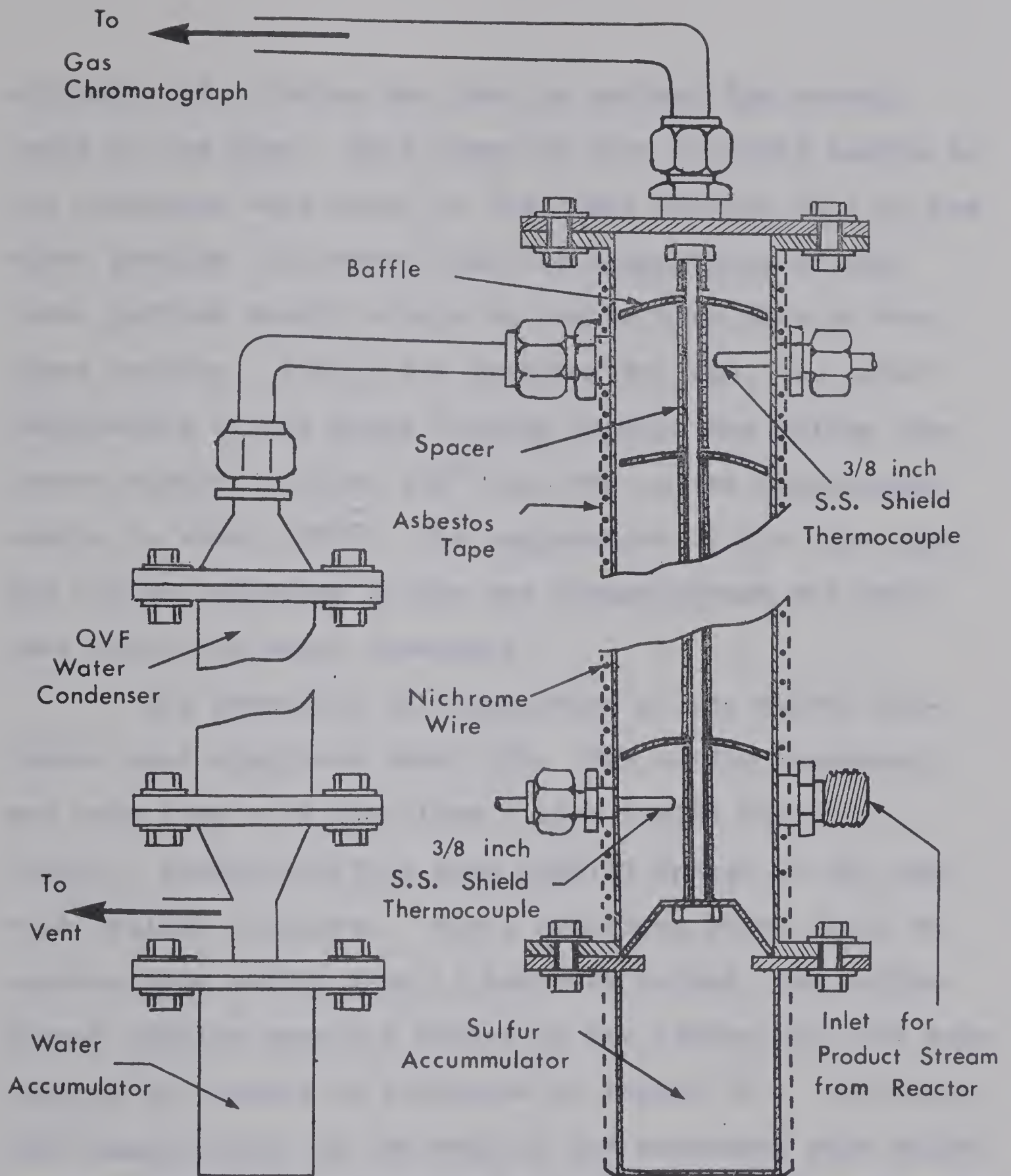


Figure 15 Modified Water and Sulfur Condensers

windings and a Variac was used to control the current input to the wire. More turns of wire per unit length of the condenser were wound on the lower portion than on the upper portion to ensure that the temperature of the lower portion should always be higher than that of the upper portion. During the experimental run, the inlet temperature of the gases flowing through the sulfur condenser should be about 350°F and the outlet temperature should be about 230°F . The temperature of the line from the sulfur condenser to the gas chromatograph was kept just above the water dew-point.

All materials of fabrication of the sulfur condenser used stainless steel 316. The sulfur condenser was made from a $1\frac{1}{2}$ foot long 1 inch inside diameter tubing. Sixteen baffles were equally spaced in the vertical sulfur condenser. Since stainless steel tends to corrode more easily when it has been welded, the convex-shaped baffles were not welded to the central bar but were secured by spacers as indicated in figure 15 . Similarly, the flange plates at the ends of the condenser were welded from the outside. Two holes were drilled on every baffle plate. The center of $1/8$ inch diameter hole was located at $1/4$ inch from the center of the baffle plate and the distance between the edge of the baffle plate and the

center of $3/16$ inch diameter hole was $1/4$ inch. The clearance between the condenser wall and the edge of baffle plate was $1/32$ inch . It was anticipated that condensed liquid sulfur would flow downwards through the $3/16$ inch diameter holes near the edge of the baffle plates and gases would flow countercurrently through the $1/8$ inch diameter holes near the center bar. The cup-shaped sulfur accumulator, at the bottom of the condenser, was 1 inch in diameter and 3 inch in length. The inside diameter of the flange plate of the sulfur accumulator was less than one inch. A tripod-shaped support was bolted to the lower end of the center bar of the baffle plates. The support stood on the small edge of protrusion formed by the flange plate of the sulfur accumulator along the wall of the condenser. Condensed sulfur would flow through the large openings between the legs of the tripod-shaped support into the accumulator. This picture can be better understood after seeing figure 15 .

Experimental runs proved that the performance of the modified sulfur condenser was satisfactory because no plugup problem occurred. When the sulfur accumulator was almost filled with sulfur it could be removed from the sulfur condenser for cleanup and replaced with an empty

one. The replacement required a very short time thus the heating of the sulfur condenser need not be interrupted during the replacement.

The gases leaving the sulfur condenser, nearly free of traces of sulfur, were divided into two portions. The smaller portion passed into the gas chromatograph for analysis and the larger portion entered the water condenser. The QVF glass water condenser was packed with glass wool. In the original water condenser, the exit, which was located at the bottom of the condenser, was connected directly to the vent line enabling condensed water to flow by gravity into the bottom of the condenser. In turn, the water was then carried into the vent line. The unconverted reactants would be catalyzed by water to form elemental sulfur in the vent line with resulting blockage of gas flow.

A water accumulator was connected to the bottom of the modified water condenser enabling the condensed water, removed by glass wool packing, to flow into the water accumulator while gases passed through a side opening to the vent line. This is shown in figure 15 .

4.4 Process Measurements

All measurements taken by process instruments were transformed into electric signals which were transmitted to chart recorders. Temperatures of the catalyst bed, reactor wall, fluidized bath, inlet and outlet of sulfur condenser, gas chromatograph oven, and feed were all measured separately by stainless steel-shielded iron-constantan thermocouples.

The millivolt signal from the thermocouple was adjusted by an Acromag model 323 electronic 0°C reference and then measured by a Honeywell 24 point Elektronik 16 millivolt recorder. The recorder was equipped with an integral solid state calibrator, chart span selector (5 millivolts to 5000 millivolts span), and a 0 to 1000 millivolts range suppressor. The accuracy of the recorder which was usually operated with a 5 millivolt span was regularly checked with a calibrated Leed and Northrup model 8686 millivolt potentiometer. The electronic zero reference unit was occasionally checked against an ice bath. The pressure and flow-rate of the feed stream were measured by a Foxboro model 66FR-2 electronic absolute pressure transducer and by a Foxboro model 613DL electronic differential pressure cell, originally in the form of pneumatic signals. The reactor pressure was measured

by a stainless steel high temperature Statham absolute pressure transducer. A Foxboro 610 AR power supply was necessary for both the feed pressure transducer and differential pressure cell. The reactor pressure transducer was powered by a Kepco KG-25-0.2 power supply unit and interfaced to the recorder through a Foxboro 693 AR emf to current converter. A Foxboro 6430 HF electronic consotrol three pen recorder received these 10 to 50 milliamperere range process signals and plotted them on chart paper as percentage readings.

Before each experimental run, the calibrations of all devices used for process measurements were carefully checked.

4.5 Experimental Procedure

This section describes the essential steps performed in one experimental run. Although the experimental procedure for the reaction between H_2S and SO_2 was slightly different from that for the reaction between COS and SO_2 (involving different number of feed streams), the principal steps have remained the same. For illustration, the experimental run for the reaction between H_2S and SO_2 was chosen.

4.5.1 Operation of the Experimental Equipment

Before any experimental runs were performed, the

gas chromatograph heated compartment should be continuously heated at a constant temperature for more than twelve hours. Stable thermal conditions for the gas chromatograph column and thermal conductivity detector cell were necessary in order to obtain good gas chromatographic analysis. Flow rates of the helium carrier and the reference gas should be checked and adjusted to the required level. Usually, a stable base-line indicated stable conditions for the gas chromatograph.

After loading a fresh weighed batch of catalyst into the reactor, the reactor was reconnected to the recycle loop. All joints were coated with an anti-seizing agent (Silver Goop) before joining. When all parts of the recycle loop had been checked for proper fitting, a bubble leak test was conducted by using "snoop". The recycle loop and reactor assembly was then enclosed within the fluidized sand bath compartment which in turn was thermally insulated. Sand was poured into the compartment to be fluidized after air was introduced.

The fluidized sand bath was used as a heat transfer media for heating up the complete reactor, recycle loop, and feed system. The air was preheated by passing through two preheaters before entering the fluidized sand bath, as shown in figure 16. After the sand was properly

fluidized, the air heaters were turned on. At the same time, current was supplied to twelve strip heating elements mounted vertically on the wall of the fluidized sand bath compartment enabling better reactor temperature control. The temperature of the air heater was controlled by Foxboro model SGT-711-KP temperature controller and the temperature of the fluidized sand bath compartment was controlled by Honeywell model PWO5-RGM temperature controller. A sufficient flow of cooling water around the shaft of the recycle pump should also be ensured. The detailed description of the construction of the fluidized sand bath, preheaters and recycle pump has been presented [53]. Usually, two hours were required for the temperature to reach a steady state. The operation of the equipment during a kinetics measurement will be mentioned in part 4.5.3.

4.5.2 Pretreatment of Catalysts

Since the catalysts had generally been exposed to open atmosphere before use, contaminants were liable to be adsorbed on the surface and some catalyst pretreatment was needed.

The catalyst was heated continuously at approximately 500°F in the reactor for at least 24 hours. Dry

nitrogen was passed through the catalyst without recirculation during this period of time to drive away the combined water and other volatile adsorbate on the catalyst because water was believed to catalyze the reaction.

4.5.3 Kinetics Measurement

Before a kinetics run was conducted, the calibration of process measurement devices was carefully checked. Then, the product line and sulfur condenser were heated and nitrogen was introduced into the system to check the proper flow through each component of the system. After inspection for smooth rotation, the recycle pump was switched on. Continual observation of the pump during its operation is recommended. The proper operation of gas chromatograph, for analyzing either feed or product, should also be carefully checked. Usually, the change in analysis from feed to product or vice-versa could easily perturb the process flow and pressures. Such problem could be overcome by adjusting the valves controlling the flow of feed and product streams to the gas chromatograph. Reactants were introduced when all process conditions appeared steady. Minor adjustments on the process flow and metering devices were required after introduction of

the reactants. Such adjustments were relatively easy because the amount of reactants was small compared to that of nitrogen. Temperature measurements should be carefully watched when reactants were being circulated through the reactor and products were formed. A sharp rise of catalyst bed temperature was always noted when reactants entered the catalyst bed because the reaction is highly exothermic. Temperature controllers should be readjusted so that all process temperatures stayed constantly at fixed preset levels.

Feed and product streams were then analyzed by gas chromatograph until consecutive reproducible results for both the feed and product compositions were obtained. If the feed compositions and product compositions remained unchanged, it was assumed that reaction had reached a steady state and the experimental data, which included the reaction temperature, pressure, feed flow rate and compositions of feed and product streams, etc. were recorded. To ensure the steady catalytic activity during the kinetics measurements, the kinetics data recorded should be compared to those taken after the reaction had been allowed to proceed for an extended period of time (12 hours in the present studies) under a same set of reaction conditions.

4.5.4 Shutdown Procedure for Experimental Equipment

After completion of a series of kinetics runs, nitrogen alone was left flowing for about an hour to purge remaining reactants and products. The recycle pump was kept running during this period of time. Then, the recycle pump and all gas flow and heaters were switched off. However, during the cooling process, air was kept flowing through the fluidized sand bath and water was maintained circulating through the shaft seal of the recycle pump. Inspection of various parts of the equipment for preventive maintenance was performed on termination of each series of kinetics runs.

4.6 Materials

4.6.1 Gases

The COS was obtained from J.T. Baker Co., Phillipsburg, U.S.A. and all other gases used in the present studies were obtained from Matheson Co. with the suppliers' specified purities as shown below:

N ₂	99.996 %	(prepurified grade)
SO ₂	99.98 %	(anhydrous grade)
H ₂ S	99.50 %	(C.P. grade)
CO ₂	99.80 %	(Bone dry grade)
COS	99.60 %	

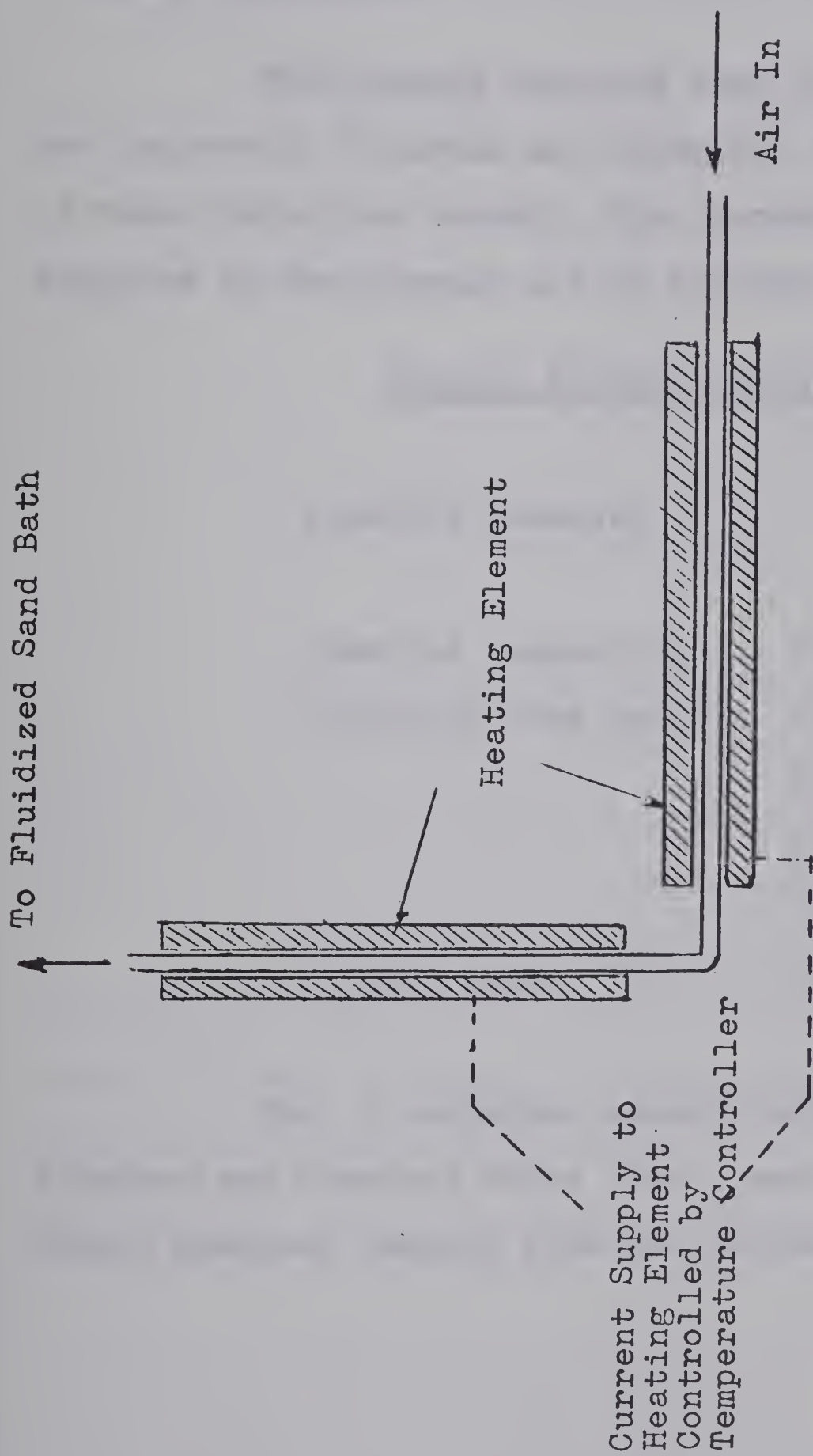


Figure 16 Air Preheater

4.6.2 Catalysts

The bauxite catalyst used in this investigation was donated by Minerals and Chemicals Philip Corporation of Menlo Park, New Jersey. The properties of the catalyst supplied by the company are as follows:

Porocel Sulfur Recovery Catalyst

Volatile material		6.0 %
Chemical composition	Al_2O_3	89.0 %
(volatile free basis)	Fe_2O_3	5.0 %
	TiO_2	2.8 %
	SiO_2	2.6 %
	Insoluble	0.6 %
Surface area	215 m^2/gm	

The γ -alumina, manufactured by Kaiser Aluminum and Chemical Sales Inc., was obtained from the Travis Chemical Company with the following properties:

KA-201 Active Alumina

Surface Area	380 m ² /gm	
Chemical composition (dry basis)	SiO ₂	0.02 %
	Fe ₂ O ₃	0.02 %
	TiO ₂	0.002%
	Na ₂ O ₃	0.30 %
	Al ₂ O ₃	93.60 %
Loss on ignition		6.00 %

Sodium-Y zeolite was obtained from the Linde Division of Union Carbide Corporation (lot SK40), hydrogen-Y zeolite was prepared by treating sodium-Y zeolite with 1 M NH₄Cl solution and dried and 500°C.

The modified catalysts used in the present studies were prepared by adding the required percentage by weight of NaOH solution (0.05 N) to the catalysts and then evaporated at 110°C for 12 hours.

4.7 Calculation of Kinetic Results from Laboratory Measured Data

The feed and product compositions were calculated from the results of the gas chromatogram peak areas by a linear least square fitted equation shown in Appendix A- V. The feed flow rate was calculated from the data obtained by the differential pressure cell by a second order equation derived from the least square fitting of the original calibration data as shown in Appendix A-IV. The reaction temperature and pressure were also calculated by substituting the recorder measurements into the equations derived from the linear least square fitting of the original calibration data as shown in Appendix A-I.

Assuming ideal gas behavior [53], the molar feed rate of nitrogen and reactants could be found from the calculated results of feed composition and flow rate. Since nitrogen is an inert, its molar flow rate should be the same in both feed and product streams. From the calculated results of the nitrogen flow rate in product stream and the product stream composition, the molar flow rate of the reactants in the product stream could also be found. The difference between the

molar flow rates of a reactant in the feed and product stream should be the rate of conversion of that reactant. Since the conversion of reactant per pass through the catalyst bed was small (differential bed reactor), it was assumed that the composition in the product stream was the same as that of the gases over the catalyst bed. This assumption has been justified [53]. It follows that the average partial pressure of each component in the gaseous phase over the catalyst could be calculated from the product compositions and the total pressure in the reactor.

A computer program called H2SSO was used to process the experimental raw data into calculated rates of reaction of H_2S and SO_2 . This program is listed in Appendix E-I. Another computer program called COSSO was used to process the experimental raw data of the reaction between COS and SO_2 into corresponding reaction rates. This program is also listed in Appendix E-I

A detailed description of the calculation method mentioned here is shown in Appendix D.

CHAPTER 5

EVALUATION OF DIFFERENT CATALYSTS FOR THE REACTION
BETWEEN H_2S AND SO_2

In industrial modified Claus process sulfur plants, the reaction conditions between H_2S and SO_2 (usually in a 2:1 molar ratio) in the catalytic converter are summarized below:

Temperature (°K)	Pressure (atm)	Space Velocity ($\frac{\text{std ft}^3}{\text{ft}^3 \text{ cat.}}$)	Reactant Composition (mole %)	
			H_2S	SO_2
480 to	slightly	650 to	1 to	0.5 to
560	above 1	960	5	2.5

The performance of various industrial catalysts towards the reaction between H_2S and SO_2 can be evaluated over a very wide range of reaction conditions. It is possible for a catalyst which exhibits poor performance at one set of reaction conditions to exhibit a superior performance at another set of reaction conditions. In the present work, it was hoped that the operation of the catalytic reactors of industrial sulfur plants could be improved by using catalysts which exhibited superior performance in catalysts evaluation tests. As a result, to evaluate alternative catalysts it was decided to compare

their catalytic performance on the basis of the extent of reaction between H_2S and SO_2 which was attained over a range of reaction conditions similar to those encountered in industry. Actually, the comparison of catalytic performance is more valid when carried out on a long-term test basis but practically, because of the limitations of time and laboratory equipment endurance, it can only be done over a short-term period (a few days) in the present studies.

5.1 Kinetic Measurements

The reaction conditions used to measure the kinetics of the reaction between H_2S and SO_2 over the seven different catalysts are summarized in table 5.1. The results of the kinetic measurements are listed in detail in Appendix E-IV showing the product stream compositions, the partial pressures of various components in the reactor, etc. As can be seen in Appendix E-IV, by varying only the feed flow-rate within the chosen range, seven different kinetics measurements were carried out for each catalyst. For each measurement, the space-time, $W/F\text{H}_2\text{S}$, where W is the weight of catalyst (gm) and $F\text{H}_2\text{S}$ is the volumetric flow-rate of H_2S in feed (std ft^3), was calculated and plotted versus percentage conversion of H_2S as shown on figure 17. The results shown in Appendix E-IV were calculated using a computer program

TABLE 5.1 REACTION CONDITIONS FOR CATALYSTS EVALUATIONS

Type of Catalysts	Tempe- rature (°K)	Press- ure (atm)	Feed Flow rate (SCFH) from to	Catalyst weight (gm)	Feed Composition (mole %) N ₂ H ₂ S SO ₂	H ₂ S conversion (%) from to
2% doped γ-alumina	510	1.13	11.42 48.53	1.24	95.31 3.11 1.58	45.27 68.87
5% doped γ-alumina	510	1.13	11.36 49.28	1.24	95.34 3.09 1.57	43.49 67.62
γ-alumina	510	1.13	11.28 48.80	1.24	95.23 3.16 1.61	37.51 57.38
2% doped bauxite	510	1.13	11.23 48.61	1.24	95.07 3.27 1.66	34.15 54.82
bauxite	510	1.13	11.23 48.61	1.24	95.07 3.27 1.66	30.19 44.46
Na-Y zeolite	510	1.13	11.33 48.73	1.24	95.28 3.08 1.54	10.20 25.39
H-Y zeolite	510	1.13	11.12 48.55	1.24	95.42 3.05 1.53	8.24 23.93

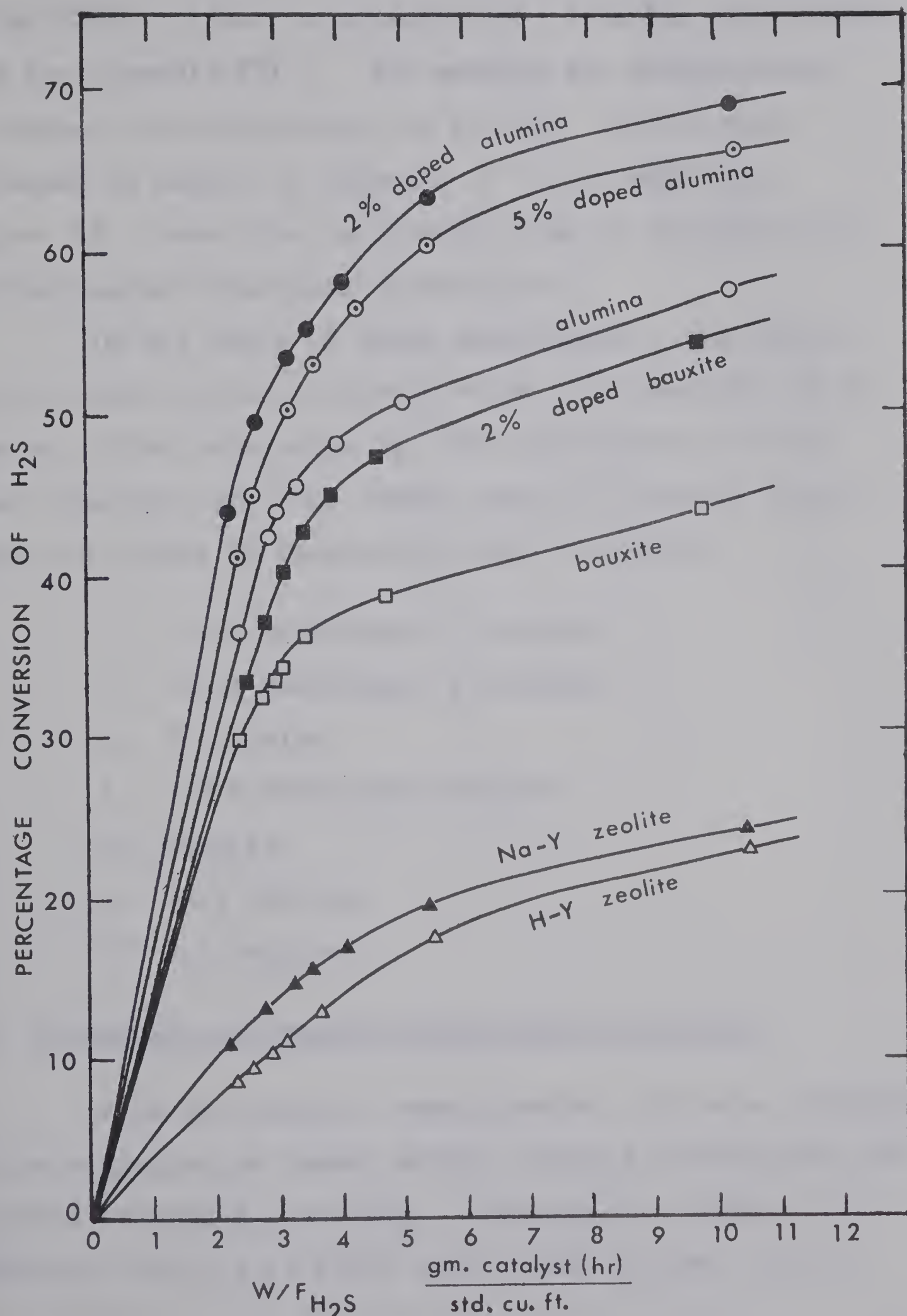


Figure 17 Comparison of Catalyst Performance towards the reaction between H_2S and SO_2

called H2SSO (listed in Appendix E-I) from the experimental data (in Appendix EII). The methods and step-by-step procedures for calculating the kinetic results were explained in detail in Appendix D . In addition, figure 18 shows the calculated rates of reaction also plotted against fractional conversion .

On the basis of these measurements, the performance of the various catalysts shown in figure 17 can be seen to differ substantially. The performances of the seven catalysts over the chosen range of reaction conditions are ranked in descending order as follows,

1. 2.0 % NaOH-doped γ -alumina
2. 5.0 % NaOH-doped γ -alumina
3. γ -alumina
4. 2.0 % NaOH-doped bauxite
5. bauxite
6. Na-Y zeolite
7. H-Y zeolite

5.2 Discussion on Catalyst Performance Variations

From the kinetic measurements, all seven catalysts are to a greater or lesser extent active in catalyzing the reaction between H_2S and SO_2 . Although the "source" of catalytic activity is still unknown and further study is

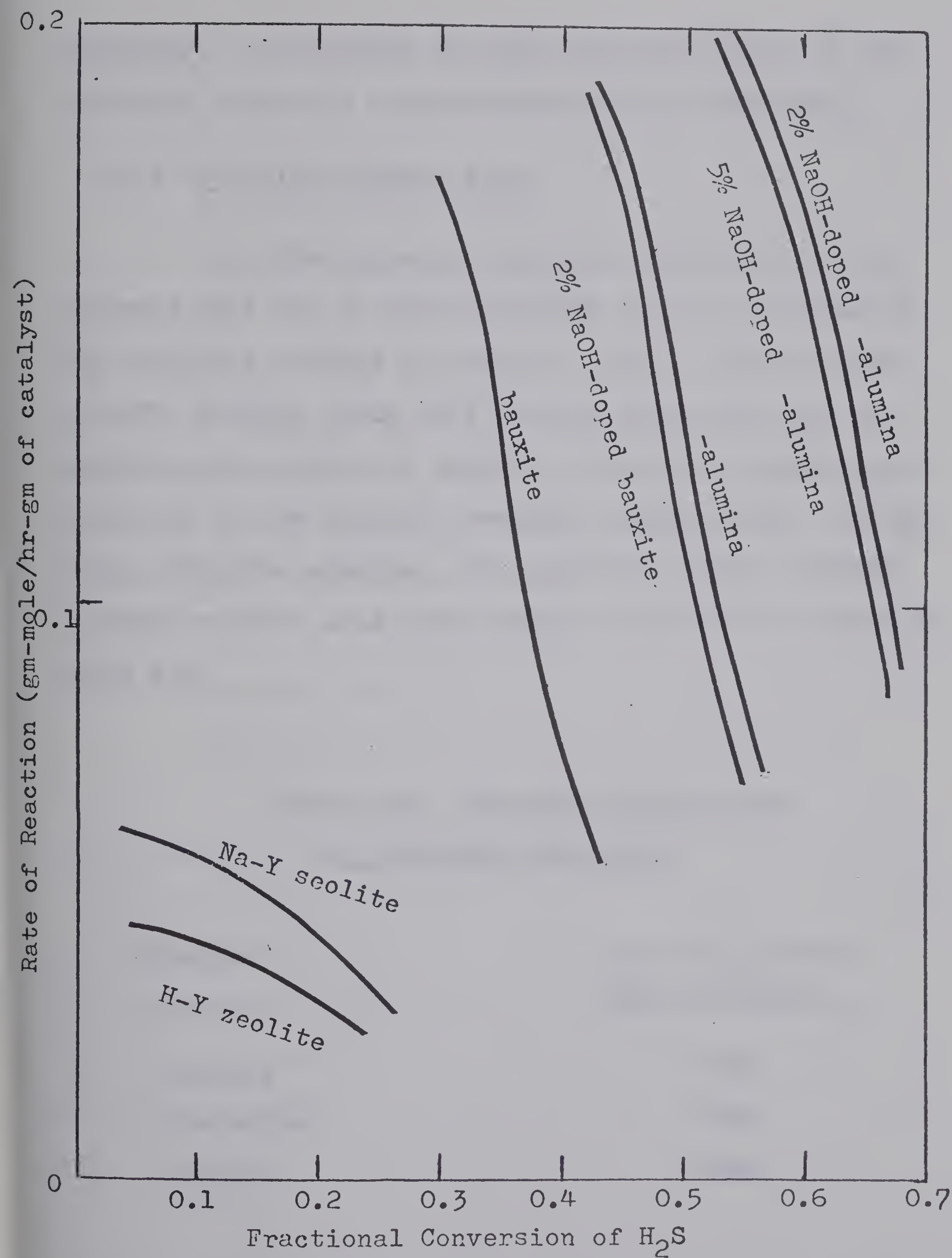


Figure 18 Rate of reaction between H_2S and SO_2 at different conversion

necessary, a discussion on some possible causes of the different catalytic performances will be presented.

5.2.1 Specific Surface Area

In heterogeneous catalytic reactions, it is believed that one or more reactants must be adsorbed on the catalysts surface in order to react. Since larger specific surface areas will provide more sites for adsorption, the extent of reaction should be somewhat proportional to the catalyst specific surface area. Of the seven catalysts examined, the zeolites usually exhibit a larger surface area than alumina or bauxite as shown in table 5.2.

Table 5.2 Specific Surface Area
of Different Catalysts

<u>Catalyst</u>	<u>Specific Surface Area (m²/gm)</u>
bauxite	215
Y-alumina	380
zeolite	640

If the function of these catalysts is merely to bring the H_2S and/or SO_2 into contact on the surface regardless of the chemical properties of the catalysts, zeolite, with the largest surface area, should exhibit the highest initial catalytic activity towards the reaction between H_2S and SO_2 . From the results of the kinetics measurements, zeolite provides the least conversion for the reaction between H_2S and SO_2 . Therefore, it appears that some surface "chemical groups" or "sites" which may be essential in adsorbing H_2S and SO_2 on zeolite are lesser in population than those on alumina or bauxite.

5.2.2 Possible Adsorption Mechanisms Responsible for Causing Difference in Catalytic Performance

From the previous work [23] using the infrared spectroscopic technique on the adsorption of H_2S and SO_2 on both γ -alumina and zeolite, it was believed that both H_2S and SO_2 formed hydrogen bonding with the 3785 cm^{-1} IR vibration frequency hydroxyl group of the catalysts. The other two hydroxyl groups of the catalysts exhibit IR vibration frequencies at 3720 cm^{-1} and 3680 cm^{-1} . Moreover, it was also found that zeolites contained very small amounts of surface hydroxyl groups compared to those on alumina and bauxite. These observations may be used to

explain why zeolites are less active towards the reaction between H_2S and SO_2 . On the other hand, from the results of the kinetics measurements, both NaOH-doped γ -alumina and NaOH-doped bauxite exhibited higher catalytic activity than their undoped counterparts even though it has been shown that NaOH-doping results in decreased specific surface area [15]. This previous work [15] also showed that when the γ -alumina was 1.0% doped with NaOH, the 3785 cm^{-1} surface hydroxyl group disappeared and when it was 5.0% doped with NaOH, both the 3785 cm^{-1} and 3680 cm^{-1} disappeared, presumably forming the structure $=\text{Al}-\text{O}-\text{Na}$. The NaOH-doped γ -alumina has fewer surface hydroxyl groups than the undoped catalyst, yet it is more active towards the reaction between H_2S and SO_2 . Therefore, the reaction between H_2S and SO_2 may not be considered as simply involving the formation of the hydrogen bonding of H_2S and SO_2 to the surface hydroxyl groups. The sodium ions on the doped catalyst surface may have played a role in catalyzing the reaction between H_2S and SO_2 . On the basis of this possibility, two postulated adsorption mechanisms of H_2S and SO_2 on the NaOH-doped catalysts can be considered. A comparison on which mechanism is the more probable will be discussed:

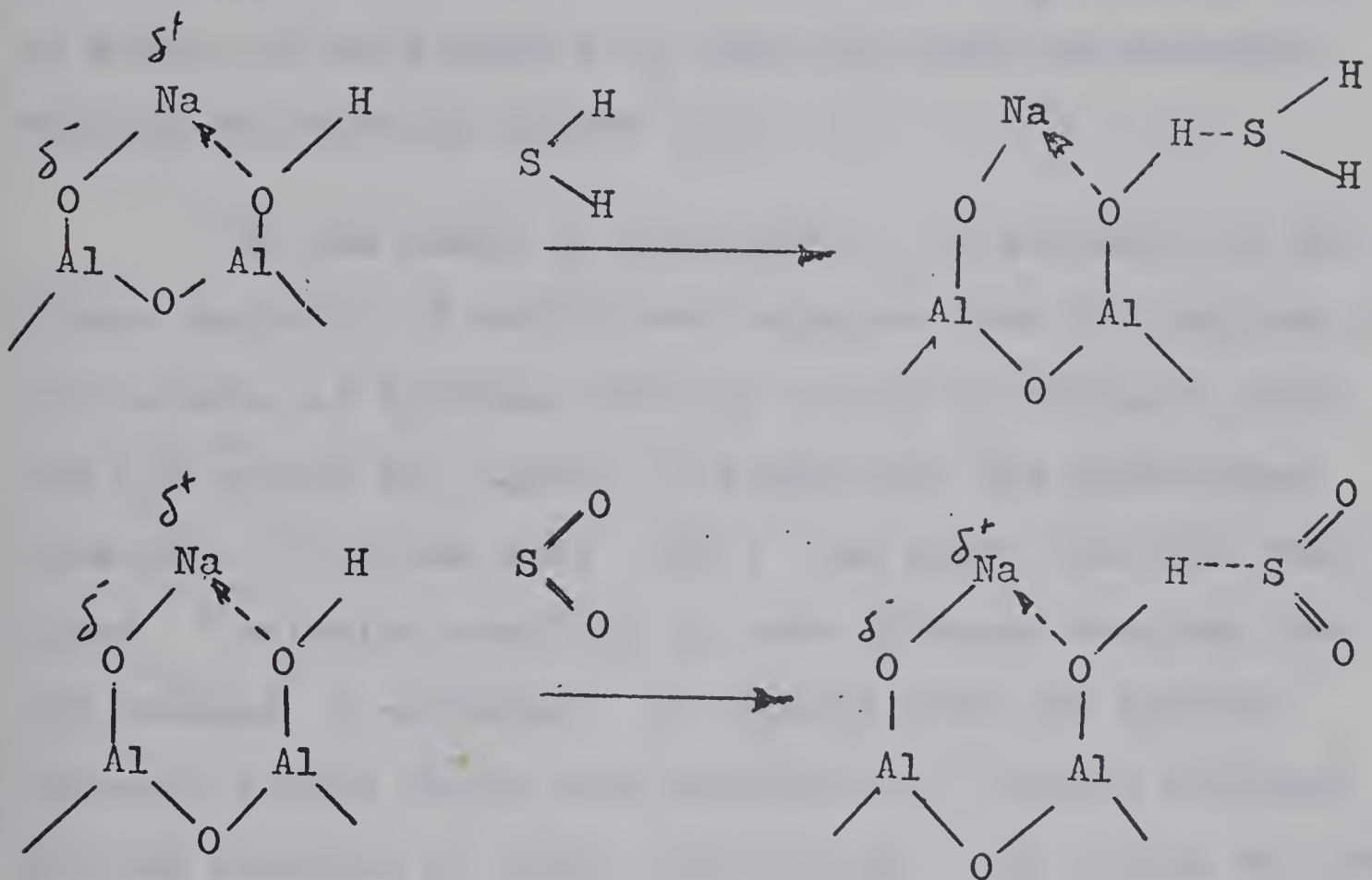
Mechanism I

The group $-O-Na$, formed from the reaction between $NaOH$ and a surface hydroxyl group does not take part directly in the adsorption. The adsorption of H_2S and SO_2 still takes place via hydrogen bonding with the surface hydroxyl group. As mentioned earlier, only the 3785 cm^{-1} hydroxyl group formed hydrogen bonding with H_2S and SO_2 and when the catalyst was 1.0 % doped with $NaOH$, the 3785 cm^{-1} hydroxyl group was removed. Since the amount of $NaOH$ used for catalyst doping in the present studies was more than 1.0 %, no 3785 cm^{-1} hydroxyl group should be expected to remain after $NaOH$ doping. It is postulated herein that due to the great difference in electronegativity between sodium and oxygen, the $-O-Na$ group may be expected to have partial ionic character. This may influence the 3720 cm^{-1} and/or 3680 cm^{-1} hydroxyl groups to become "acidic" and thus result in hydrogen bonding formation as shown in figure 19 .

Mechanism II

The group $-O-Na$, expected to have partial ionic character, will be partially positive in charge on sodium with respect to the oxygen. This sodium end will then be expected to be electrophilic and will thus be capable of attracting

Mechanism I



Mechanism II

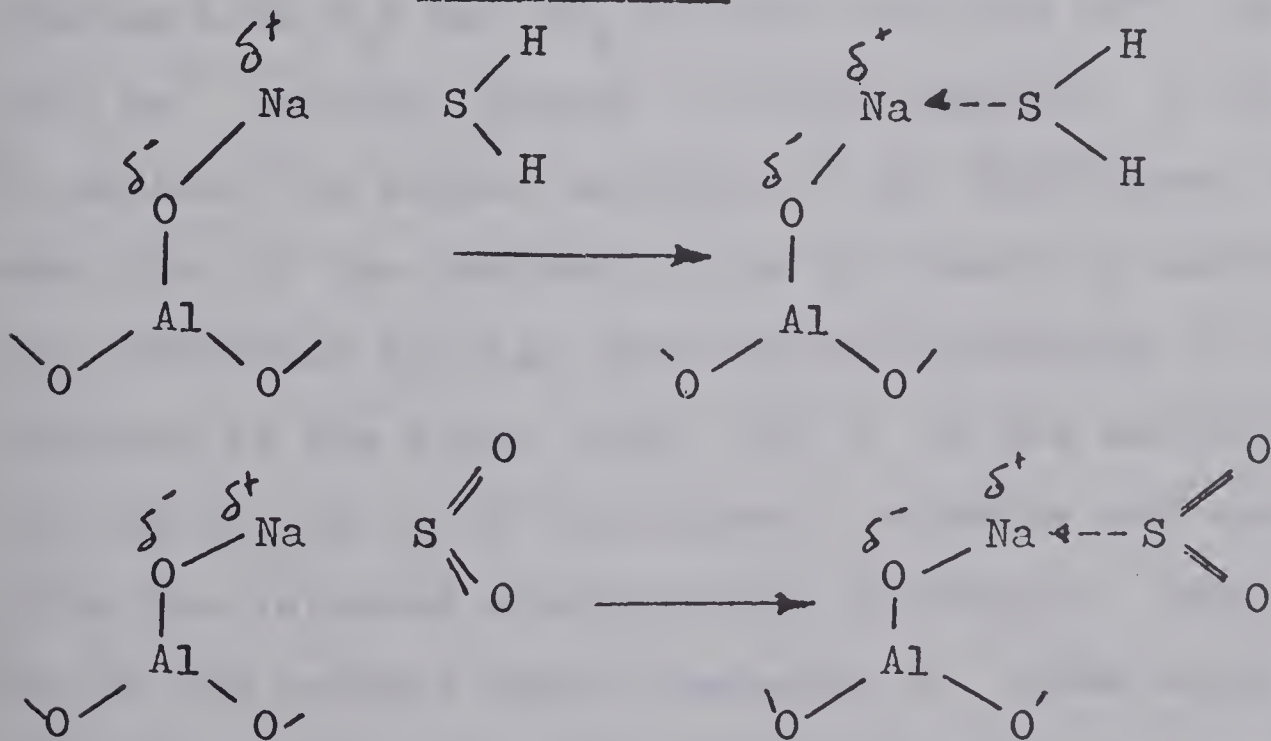


Figure 19 Proposed Adsorption Mechanism of H_2S and SO_2 on Gamma alumina. doped with NaOH

unshared electrons in the sulfur atom of H_2S or SO_2 . In so doing, it will adsorb H_2S and SO_2 onto the catalyst surface as shown in figure 19 .

On the basis of mechanism I, to account for the higher activity of NaOH-doped catalyst over the undoped one, the amounts of hydrogen bonding formed by hydroxyl group and H_2S and/or SO_2 should be higher for the NaOH-doped catalyst. Previous work [23] has shown that the NaOH-doped γ -alumina resulted in less hydrogen bonding than on the undoped γ -alumina. It appears that the surface hydroxyl groups which were incapable of forming hydrogen bonding remained so after NaOH-doping. The reason why only the 3785 cm^{-1} hydroxyl group is active towards hydrogen bonding with H_2S and SO_2 and not the 3720 cm^{-1} and the 3680 cm^{-1} hydroxyl groups is still unknown. It is possible to explain the higher activity of the NaOH-doped catalyst over that of the undoped one on the basis of mechanism II. The adsorption species shown as the mechanism II were not observed in the cited study [23] of the adsorption of H_2S and SO_2 on 2.0 % NaOH-doped γ -alumina and zeolite using the infrared spectroscopic technique. This may be due to the partial ionic character of $-\text{O}-\text{Na}$ which raises the vibration frequencies associated with the adsorbed H_2S or SO_2 to a level too high to be detected by the

infrared spectrophotometer with its upper frequency limit of 4000 cm^{-1} . Referring to the results of kinetics measurements shown in table 5.1, the 5.0 % NaOH-doped γ -alumina was slightly less active than the 2.0 % NaOH-doped γ -alumina. Mechanism II is unable to explain the result because the higher the sodium content of the NaOH-doped catalyst, the higher its activity should be and therefore the 5.0 % NaOH-doped γ -alumina should be about twice as active as the 2.0 % NaOH-doped γ -alumina. This seeming contradiction between mechanism II and the results of the kinetics measurements can be explained on the basis that it is the result of differences in specific surface area. Previous work [15] has shown that the surface area of 2.0 % NaOH-doped γ -alumina was reduced by 20 % and that of 5.0 % NaOH-doped γ -alumina was reduced by 70 %, when compared to that of the undoped γ -alumina. Consequently, the surface area of the 2.0 % NaOH-doped γ -alumina was about 2.7 times that of the 5.0 % NaOH-doped γ -alumina. Assuming that the total number of -O-Na groups is proportional to the extent of NaOH doping, and that the "accessible" -O-Na groups are proportional to surface area, then on the basis of mechanism II, the ratio of the conversion of H_2S by the 2.0 % NaOH-doped γ -alumina to that by the 5.0 % NaOH-doped γ -alumina

can be calculated as follows:

Total [-O-Na] of 2.0 % NaOH-doped γ -alumina

Total [-O-Na] of 5.0 % NaOH-doped γ -alumina

$$= 1/2.5$$

Accessible [-O-Na] of 2.0 % NaOH-doped γ -alumina

Accessible [-O-Na] of 5.0 % NaOH-doped γ -alumina

$$= \frac{\text{Surface area of 2.0 \% NaOH-doped } \gamma \text{-alumina}}{\text{Surface area of 5.0 \% NaOH-doped } \gamma \text{-alumina}}$$

$$= 2.7/1$$

therefore,

Conversion of H_2S by 2.0 % NaOH-doped γ -alumina

Conversion of H_2S by 5.0 % NaOH-doped γ -alumina

$$= 1/2.5 \times 2.7/1$$

$$= 1.08$$

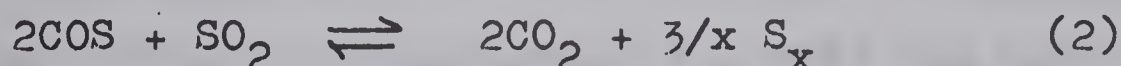
which is only slightly higher than the result shown in table 5.1. Since the differences in activity between the 2.0% and 5.0% NaOH-doped γ -alumina can be explained in terms of specific surface area, then the added 3.0% NaOH content does not appear to be significant.

Similarly the higher activity of γ -alumina over bauxite may also be explained in terms of its larger surface area. However, the difference between the activities of the pure γ -alumina and the 2.0% NaOH-doped γ -alumina cannot be explained on the basis of specific surface area since the latter, with the lower area, exhibits the greater activity. Mechanism II cannot be discounted but it also appears to be unsuitable because additional NaOH content in itself does not appear to be influential on the catalytic activity.

CHAPTER 6

KINETICS AND MECHANISTIC STUDIES OF THE REACTION
BETWEEN COS AND SO₂

Since unconverted COS present in sulfur plant stack gases frequently accounts for roughly one-third of the total sulfur losses, it is of interest to examine the possibility of converting COS to elemental sulfur. For this reason, the kinetics of the reaction between COS and SO₂ to form sulfur according to reaction (2)



was investigated over γ -alumina. Bauxite and alumina are the most commonly used catalysts in the sulfur industry. The reason why γ -alumina was chosen over the other industrial catalysts for this investigation is that pure

γ -alumina contains only Al₂O₃ whereas bauxite is a mixture of minerals, including γ -alumina. The more "pure" form of catalyst facilitates interpretation of the mechanistic studies of the reaction between COS and SO₂ since the influence of other constituents towards the reaction is minimized. Mechanistic studies of the reaction were carried out in the present work because it was hoped that such studies might offer an explanation why COS was unsuccessful

fully converted to sulfur in the industrial catalytic converter.

6.1 Kinetic Studies of the Reaction between COS and SO₂

The high thermodynamic feasibility of this reaction has already been shown. The kinetics measurements in the present study were carried out within the industrial range of conditions as shown in table 6.1.

Run 1 was tested whether the homogeneous reaction between COS and SO₂ occurred at the reaction conditions. Both feed and product chromatograms for this run were found to be identical and hence it was concluded that no homogeneous reaction occurred under that set of reaction conditions.

Run 2 represents the trial run to obtain preliminary information about the approximate rate of reaction between COS and SO₂. In this run, the reaction was allowed to proceed for more than one hour before the product analysis was performed but, this first analysis indicated that no reaction had occurred. Another similar run using the same weight of fresh catalyst was performed and similar results were again obtained. These results seemed contradictory to the high feasibility that had been anticipated for this reaction. It was suspected that perhaps the

TABLE 6.1: EXPERIMENTAL PROGRAM COS/SO₂ KINETICS

Run Number	Number of Feed and Product Analysis	Catalyst Weight (gm)	Temperature (°K)	Pressure (atm)	Feed Flow Rate (SCF/hr)	Feed Composition (mole %)		
						N ₂	H ₂ S	SO ₂
1	1	1.26	522	1.13	3.0	94.0	4.0	2.0
2	1	1.00	510	1.13	3.0	91.0	6.0	3.0
3	1	2.68	522	1.13	3.0	94.0	4.0	2.0
4	7	2.68	522	1.13	3.37	93.9	4.68	2.23
5	7	4.89	557	1.13	4.69	94.0	4.0	2.0
6	3	1.24	510	1.13	3.0	94.0	4.0	2.0

reaction rate was slow under the chosen set of reaction conditions and thus a larger quantity of catalyst might increase the conversion to a detectable amount. This led to the modification of the reactor which permitted larger catalyst charges to be used.

With the modified reactor, four kinetics runs, represented as runs 3 to 6 in table 6.1, were carried out. Run 3 tested if conversion of COS would increase to a detectable amount with increase in catalyst charge. The reaction was allowed to proceed for about 1½ hours before any product analysis was taken. Again, it was found that the chromatograms of the feed and product were identical. A further check analysis of the product gave the same results, thus the absence of reaction which was also observed in the previous runs could not be explained in terms of reactor catalyst charge limitations.

Previous results reported in the literature on the kinetics of the reaction between COS and SO₂ did not pay specific attention to the attainment of constant catalytic activity during the kinetics measurements. The high feasibility of this reaction reported by earlier workers suggested that their results may have been short-term results using a fresh charge of catalyst during the initial stage of introduction of reactants. To verify this

possibility, run 4 was performed with the first product analysis taken at 6.0 minutes after introduction of the feed. The results, shown in Appendix EV and on figure 20 indicate that conversion of COS measured by the first product analysis was 56.55 %, and thus proving that

γ -alumina was catalytically active during the early stage of reaction. The subsequent six consecutive product analyses showed that the conversion of COS dropped as the time passed and became almost undetectable after about 1½ hours of reaction. By turning off the reactant flow and leaving only pure nitrogen flowing through the system for one hour, an attempt was made to regenerate the activity of the catalyst. Unfortunately, this attempt failed and the drop in COS conversion must be attributed to some form of catalyst "poisoning". Initially, it was suspected that elemental sulfur, formed from this reaction, had condensed on the catalyst surface and hence "poisoned" the active sites of adsorption by covering them. To test for such a possibility, run 5 was performed in which higher reaction temperature was used to ensure that the dew point of sulfur vapor was not reached. The conversion of COS, as shown in Appendix E-V and on figure 20, were higher than those obtained in the earlier runs, however the reaction again came almost to a halt in about 1½ hours. Purging the system

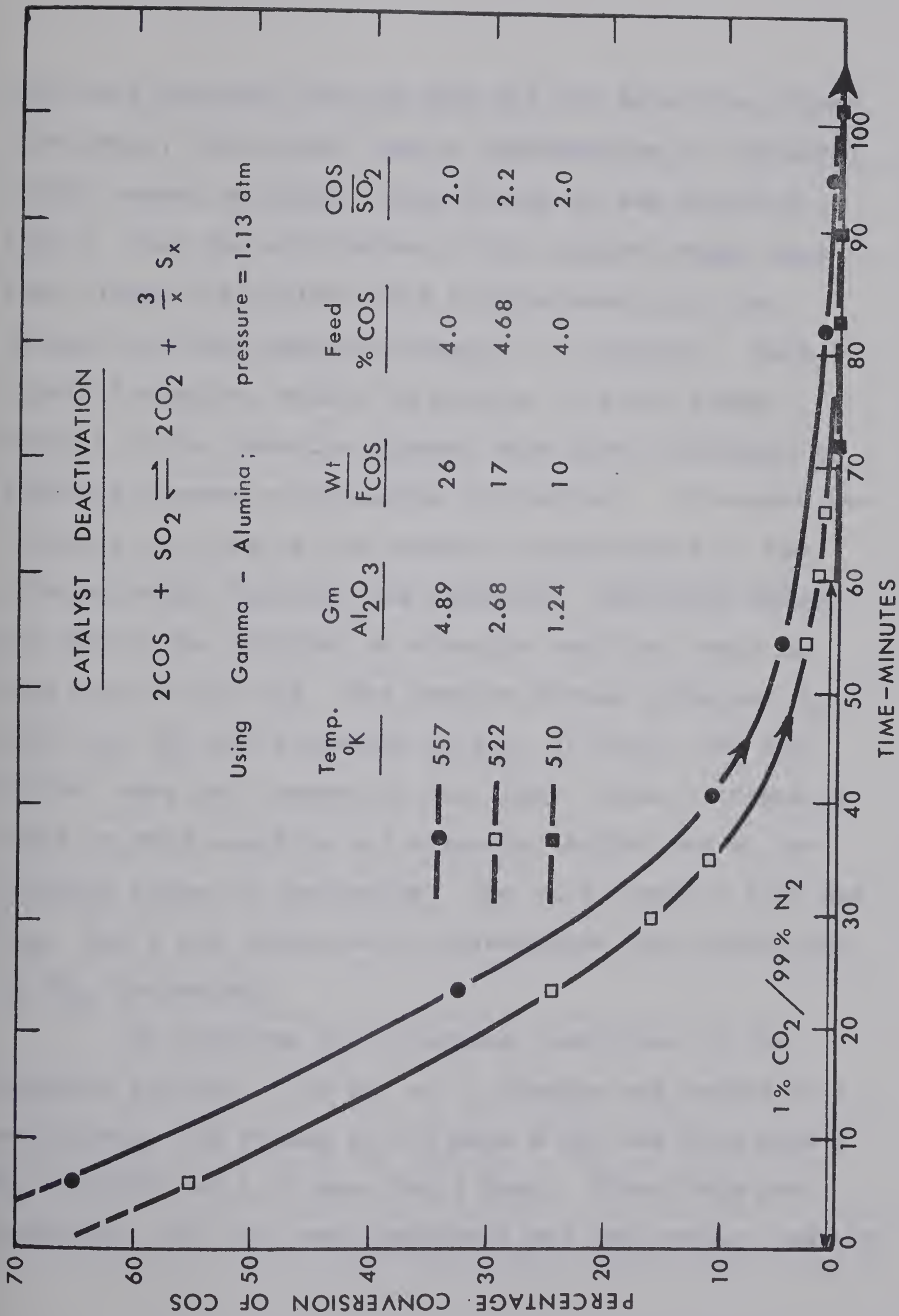


Figure 20 Deactivation of Gamma Alumina Catalyst

with pure nitrogen for one hour did not alter the situation hence, "poisoning" due to condensation of elemental sulfur seemed unlikely. Even though it was reported [50] that the micropores of the catalyst might have been plugged by sulfur, such a phenomenon could not account for the complete cessation of reaction. Each chemical species, either in gaseous or solid phases, present in the reaction system, were then considered as possible sources of catalytic "poisoning". It seemed improbable that any of the chemical constituents of the catalyst might "poison" the catalyst. Reactants should not poison the catalyst or else the reaction would not have occurred at all. The product stream contained N_2 , COS, CO_2 , SO_2 and elemental sulfur, of which, CO_2 and sulfur were not present in the feed. Since nitrogen is inert to this reaction and elemental sulfur was an improbable cause of "poisoning", the only chemical left was CO_2 . Run 6 was conducted to investigate the possibility of CO_2 "poisoning".

To simulate the poisoning conditions in the reaction process, 1.24 gm of γ -alumina was heated in a continuous flow stream of 1.0 mole % CO_2 and 99.0 mole % N_2 at $510^\circ K$ and 1.13 atm for 1 hour. After this pre-treatment, the feed was introduced and the product sampled

at 12 minutes after introduction of feed. As indicated in figure 20 , the catalyst did not catalyze the reaction after this pretreatment, suggesting that CO_2 had indeed played a primary role in the deactivation of the catalyst.

The results of the kinetics studies of the reaction between COS and SO_2 were calculated from the raw data in Appendix EIII by a computer program called COSSO in Appendix E-I . A detailed explanation of the method of calculation is shown in Appendix D .

6.2 Mechanistic Studies of the Reaction between COS and SO_2

After discovering that CO_2 had poisoned γ -alumina catalyst, it was felt necessary to study how COS reacted with SO_2 over γ -alumina to understand the influence of CO_2 . Using the infrared method [23], a gas sample was contacted with the catalyst in a glass cell fitted with a crystal NaCl window on each of its opposite ends. The cell can be connected to a conventional vacuum and gas-handling system so that gases can be introduced or removed as required. A heating section at the upper part of the cell enables wafer to be lifted up the holder into that section when thermal treatment is required. When studying the adsorption and/or catalytic reaction, the catalyst is ground to a very fine powder and then pressed into a very thin

wafer. Thinness is emphasized because a high transmittance of the IR beam through the wafer is required to increase sensitivity. The wafer is then placed in a holder in the cell and IR beam enters and leaves the cell through the NaCl windows and catalyst wafer with its path perpendicular to the faces of the catalyst wafer. Gaseous and adsorbed species in the cell can reduce the transmittance of the IR beam at frequencies characteristic to them and thus be detected.

In the present study, a Perkin-Elmer 621 high resolution double-beam infrared spectrophotometer with frequencies from 200 cm^{-1} to 4000 cm^{-1} was used.

6.2.1 Catalyst Pretreatment

The catalyst used for the present study was Alon C (from Cabot Corporation, U.S.A.), a γ -alumina with a surface area of approximately 50 to $100\text{ m}^2/\text{gm}$. About 0.1 gm of the catalyst was pressed in a stainless steel die at a pressure of around 12 tons/in^2 into a thin wafer with diameter of about $\frac{1}{4}$ inch.

The catalyst wafer was always pretreated before the spectroscopic study was carried out hence, the prepared wafer in the wafer holder was placed in the heating section of the cell. The cell was then degassed at about 400°C for

8 to 10 hours for removal of adsorbed water and volatile material. This was followed by the introduction of oxygen into the cell, and the wafer was then heated in oxygen two or three times (100 to 200 torr of oxygen each time) at about 450°C for two hours to remove traces of adsorbed organic compounds. The cell was again degassed, this time for 24 hours at about 400°C.

6.2.2 Results and Discussions

Before the IR study of the reaction of COS and SO₂ over γ -alumina was carried out the IR beam was passed through the wafer at room temperature with both sample and reference cells under vacuum to obtain a baseline spectrum for the catalyst, as shown in figure 21a. To understand the IR absorption frequencies of COS and SO₂, both in the gaseous state and in the adsorbed state over γ -alumina, about 100 torr of COS and SO₂ were contacted separately with the γ -alumina wafer at room temperature for about 2 hours. The IR spectra of gaseous COS and SO₂ were measured by lifting the wafer out of the path of the IR beam. When measuring the IR absorption for the adsorbed species on the catalyst, it is necessary to maintain the same pressure for the gas phase constituent in the reference cell as well, to eliminate interference from the

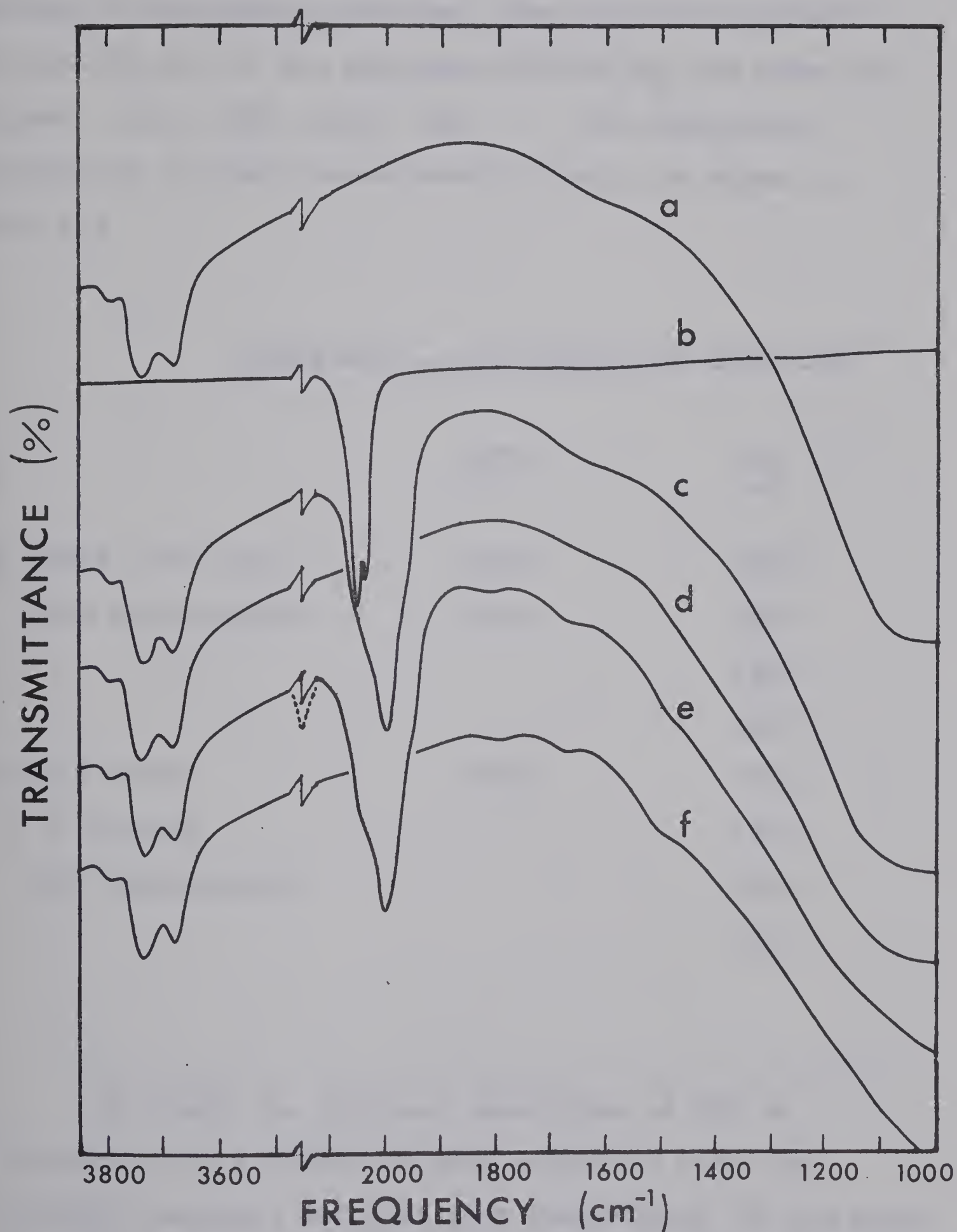


Figure 21 Spectra of COS on γ -Alumina
(a) baseline (b) Gaseous COS at room temperature
(c) exposed to 100 torr COS at room temperature
(d) degassed at room temperature (e) exposed
to 100 torr COS at 510°K (f) degassed at 510°K

gaseous IR absorption spectrum. The spectra of gaseous COS and SO₂ and of the adsorbed COS and SO₂ are shown in figures 21b, 22b, 21c, 22c . The absorption frequencies of their characteristic bands are shown in table 6.2.

Table 6.2 IR Absorption Bands, cm⁻¹

	<u>COS</u>	<u>SO₂</u>
Gas Phase (100 torr, room temperature)	2050	2499
	2070	2305
		1365
		1160
Adsorbed State (γ -alumina room temperature)	2000	1565
		1365
		1280
		1160

To study the physical adsorption of COS on γ -alumina, 100 torr of COS were contacted with the γ -alumina catalyst wafer at room temperature for one hour

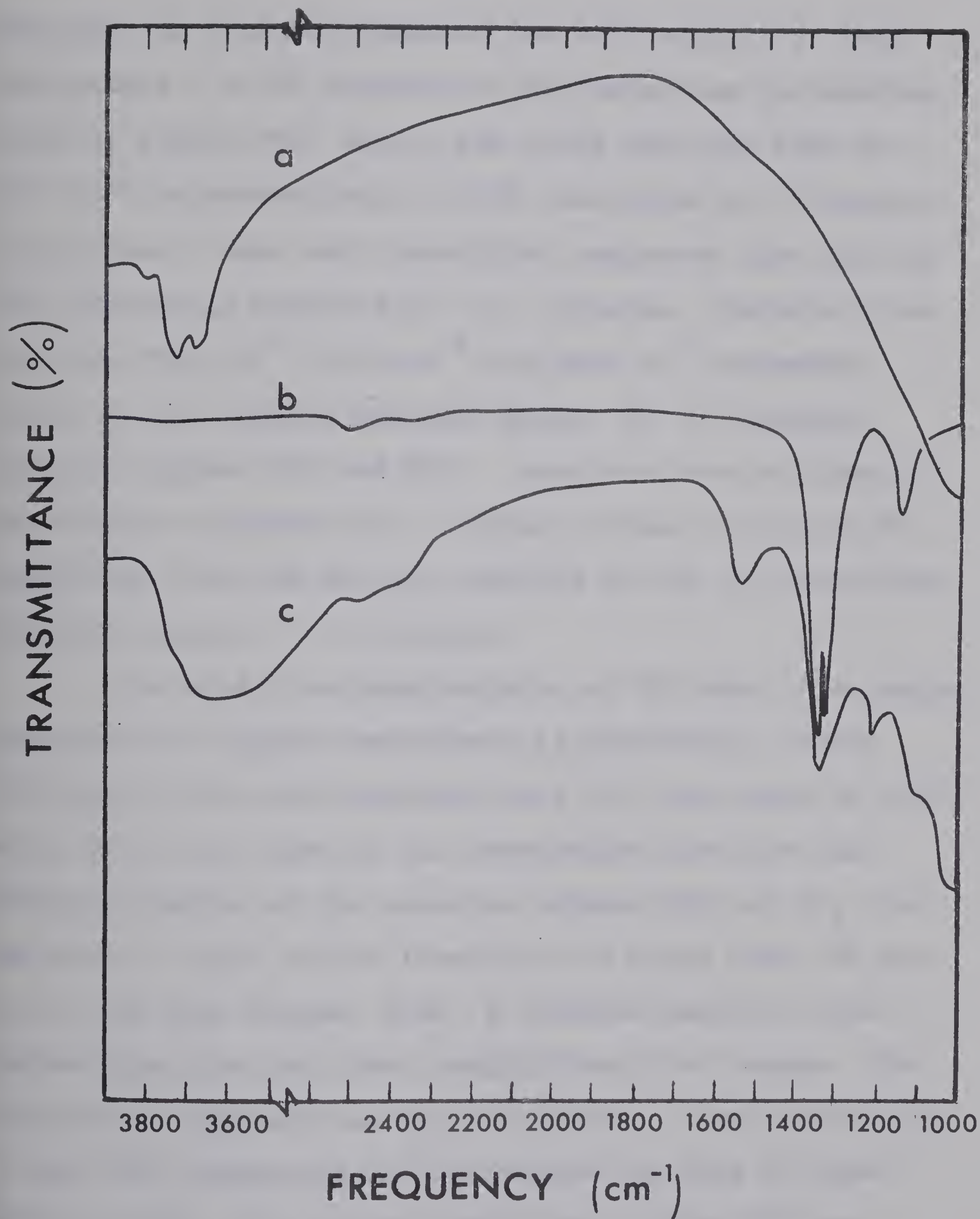


Figure 22 Spectra of SO₂ on γ -Alumina
(a) baseline (b) gaseous SO₂ at room temperature
(c) exposed to 100 torr SO₂ at room temperature

and then the cell was degassed for half an hour at room temperature. An IR spectrum of the wafer was recorded as shown by figure 21d and it was noted that the band at 2000 cm^{-1} , characteristic of COS adsorption on γ -alumina, disappeared. Such easy desorption suggested that COS was only physically adsorbed on γ -alumina. Moreover, the bands at 3785 cm^{-1} , 3720 cm^{-1} and 3680 cm^{-1} characteristic of the surface hydroxyl group of γ -alumina shown in figures 21c and 21d were the same as those of the baseline spectrum of γ -alumina shown in figure 21a suggesting that COS was not adsorbed on any of the surface hydroxyl groups of γ -alumina.

To study the chemisorption of COS over γ -alumina, exposure to a higher temperature is preferable. About 100 torr of COS were contacted with the same wafer at 510°K which is in the range of the temperature used for the kinetics studies of the reaction between COS and SO_2 for two hours. Rapid sulfur formation was noted when COS gas first came into contact with γ -alumina wafer at this temperature, but not after roughly the first minute. Two alternative explanations may be offered. One possibility is that COS decomposed on the catalyst surface to form sulfur and CO. The other possibility is that COS was oxidized by the surface oxygen on γ -alumina to form CO_2

and sulfur. The first possibility was less valid than the second because in the spectrum shown in figure 21e , taken after the cell was cooled to room temperature, the characteristic band of CO adsorption at 2200 cm^{-1} was not found whereas the CO_2 adsorption band at 2365 cm^{-1} was detected. The γ -alumina wafer used in the present studies was pretreated with oxygen and may therefore contained surface oxygen. Published references [31, 63] refer to surface oxygen on γ -alumina after oxygen pretreatment. Usually, the amount of surface oxygen on γ -alumina is small and hence the sulfur formation stopped after a very short period. This same cell was then evacuated at room temperature and a spectrum shown as figure 21f was taken. The COS adsorption band at 2000 cm^{-1} was not found in figure 21f suggesting that COS was also physically adsorbed on γ -alumina at the reaction temperature used in the kinetics measurements.

The fact that when COS was adsorbed on γ -alumina, only one band at 2000 cm^{-1} was found indicates that COS, with a structure of $\text{O}=\text{C}=\text{S}$, was not adsorbed with its carbon atom on the catalyst surface. In this situation, the vibrations of CO and CS ends would give rise to two bands or at least a doublet band. As a result, COS was

likely adsorbed through either its oxygen or sulfur atoms. From the IR absorption bands of CO_2 (2365 cm^{-1}), CO (2200 cm^{-1}) and CS_2 (1550 cm^{-1}) [909, it can be seen that the vibration frequency of CO is higher than that of CS . This is understandable because oxygen is a lighter atom than sulfur. The vibration frequency of the adsorbed COS at 2000 cm^{-1} appears to originate from the CO bond vibration rather than the CS bond vibration because 2000 cm^{-1} is closer to the vibration frequencies of CO and CO_2 than that of CS_2 , and thus COS probably was adsorbed on γ -alumina through its sulfur atom. The unshared electrons of sulfur in COS should be more easily attracted to the surface aluminum ions (Lewis-acid sites) than the oxygen atoms on the surface of γ -alumina and thus COS should more likely be adsorbed on γ -alumina through sulfur atom at Lewis-acid site.

About 100 torr of a COS and SO_2 mixture were now introduced into the evacuated cell and contacted for about 30 minutes with the same wafer at 510°K . As soon as the mixture of COS and SO_2 came into contact with the γ -alumina at this temperature, significant amounts of sulfur vapor were formed. The cell was again cooled to room temperature and the spectrum shown

in figure 23a was taken. It was found that with SO_2 present, the band at 3785 cm^{-1} disappeared with the broadening of the band at 3550 cm^{-1} appearing, suggesting that SO_2 formed hydrogen bonding with the surface hydroxyl group. The physically adsorbed CO_2 at 2365 cm^{-1} and the chemically adsorbed CO_2 at 3605 cm^{-1} , 1640 cm^{-1} and 1500 cm^{-1} were also detected.

After evacuation of the cell, about 70 torr of COS were introduced into the cell at 510°K to contact the same wafer for 15 minutes to see whether the catalyst was still active in COS adsorption. A spectrum shown in figure 23b was then taken at room temperature and indicated that the magnitude of the COS adsorption band was reduced by more than 50 % suggesting that the catalyst was less capable of adsorbing COS. In order to "poison" the catalyst faster, successive mixtures of COS and SO_2 at 100 torr were contacted with the same γ -alumina wafer followed by evacuation at 510°K .

Finally, after evacuation of the cell, about 100 torr of a mixture of COS and SO_2 gases were introduced into the same cell and an IR spectrum was taken at room temperature as shown in figure 23c. The bands at 3605 cm^{-1} , 1640 cm^{-1} and 1500 cm^{-1} characteristic of chemisorbed CO_2 were more prominent. The cell was then

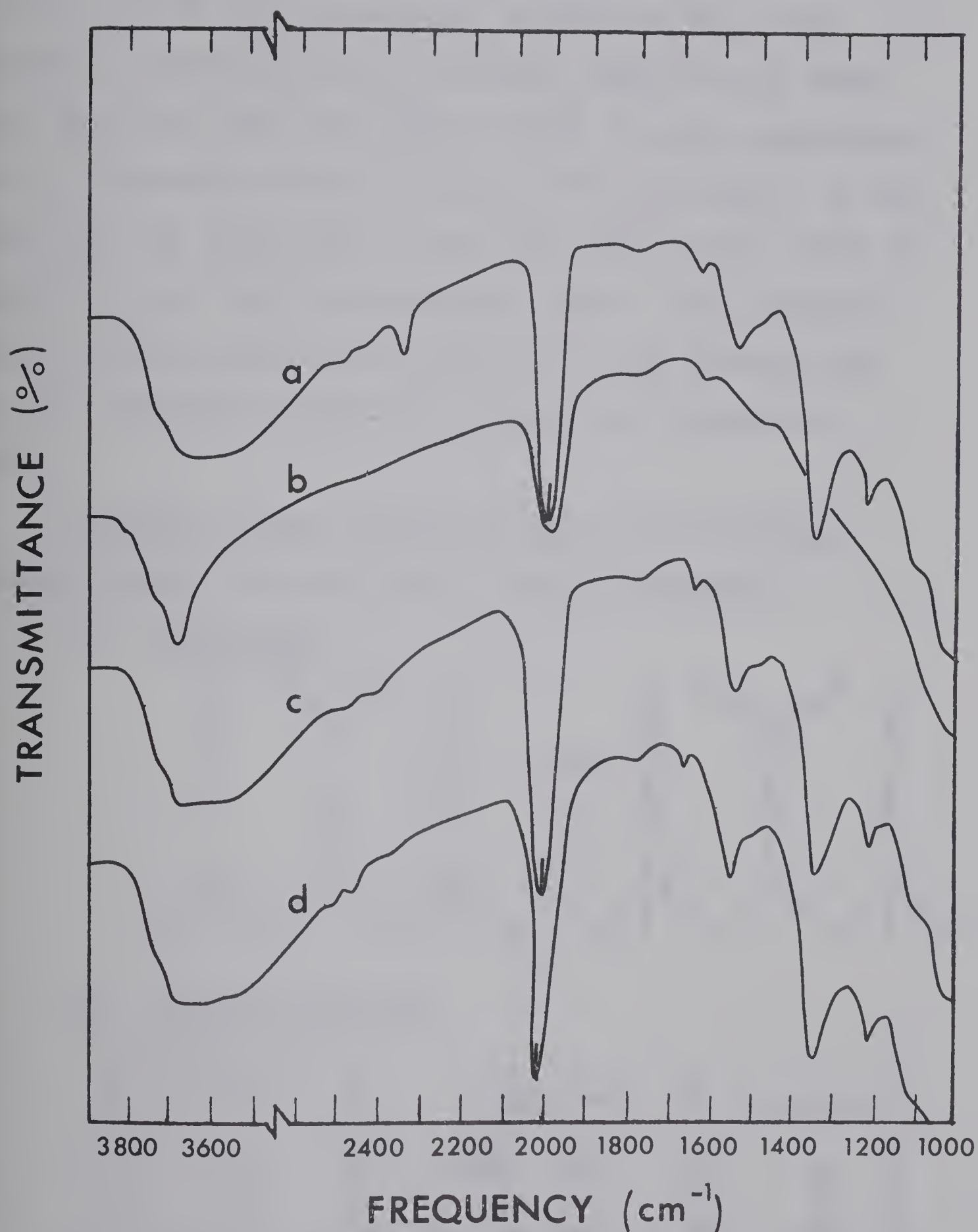
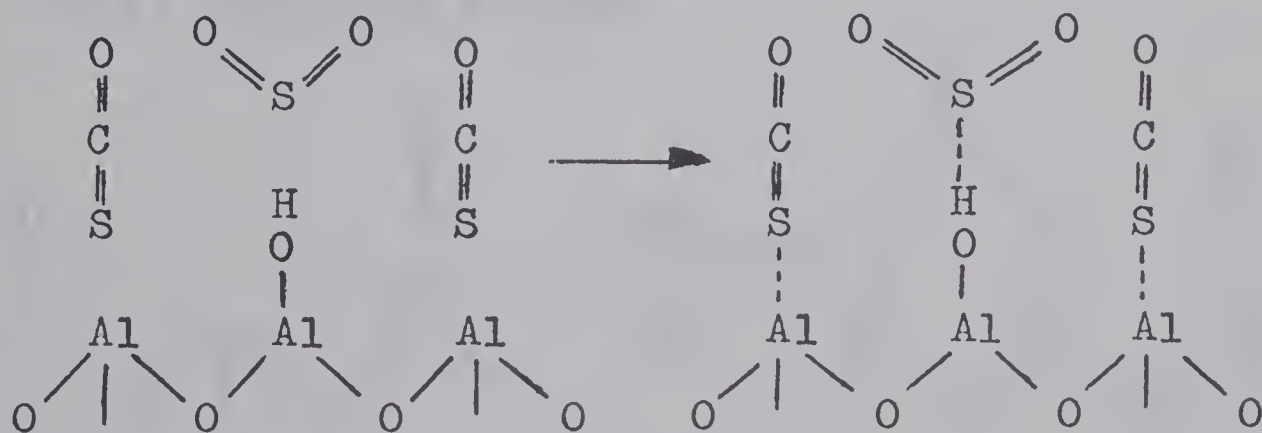


Figure 23 Spectra of COS and SO₂ on γ -Alumina
(a) COS and SO₂ reacted on catalyst surface at 510°K
(b) then degassed and exposed to 70 torr COS at room temperature (c) then degassed and exposed to 100 torr COS/SO₂ mixture at room temperature (d) after exposing for 12 hours to gas mixture at 510°K

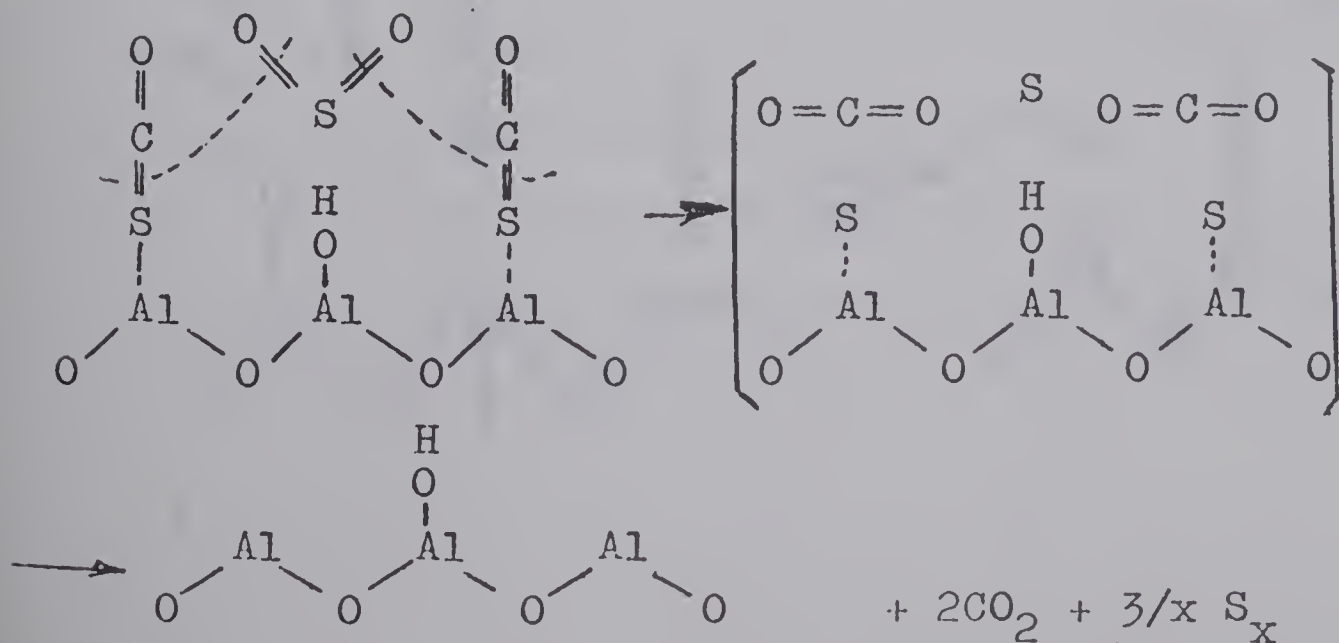
heated to 510°K and the mixture of COS and SO_2 was allowed to contact with the catalyst wafer for 12 hours after which the cell was again cooled to room temperature and an IR spectrum shown in figure 21d was taken. It was found that the magnitude of both the COS and SO_2 bands of figures 21c and 21d was nearly the same. This evidence indicates that very little reaction if any between COS and SO_2 took place during the 12 hours of contact at 510°K .

Combining these points-of-view, the following surface reaction between COS and SO_2 is proposed:

(i) Adsorption

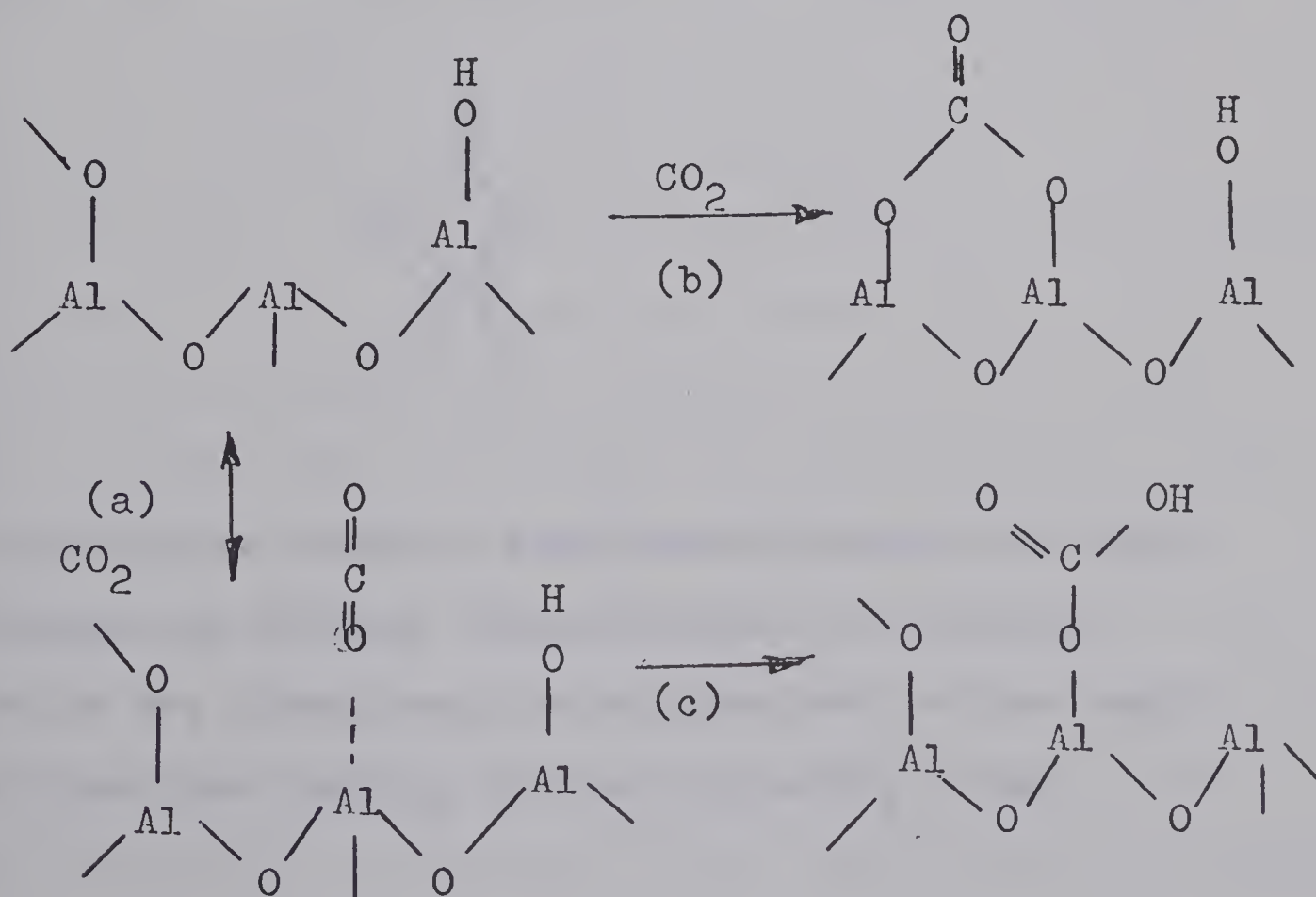


(ii) Surface Reaction

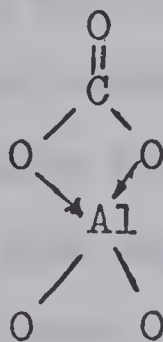


This mechanism can take into account the stoichiometric amounts of reactants shown in reaction (2). The exact reaction mechanism between the adsorbed COS and SO_2 molecules is still unknown. The sulfur formed from the reaction may be adsorbed on the catalyst surface or desorbed into the gaseous phase. This picture is still not clear. Since thermodynamically the formation of S_6 and S_8 chains is favored, these chains can form in the gas phase through recombinations between S atoms dimers, etc., or on the catalyst surface involving adsorbed S species. In this latter case, holdup of sulfur within the micropores of the catalyst may result.

(iii) Poisoning Process



Gregg and Ramsay [31] studied the adsorption of CO_2 on k-alumina using the IR technique. Adsorption bands at 2365, 1652, 1460 and 1234 cm^{-1} were found. By examining the effect of elevated temperature, i.e. 400°C , and evacuation on these bands, it was noted that the band at 2365 cm^{-1} was due to physical adsorption and the other three bands were due to chemically adsorbed CO_2 . The authors suggested that the 1460 cm^{-1} band probably originated from CO_2 present in the fine pores, in a form resembling the CO_3^{2-} ion, and that the bands at 1652 and 1234 cm^{-1} resulted from a chemisorbed bidentate carbonate ion (with structure shown below



Their adsorption isotherm measurements supported these conclusions and further indicated that the process leading to the formation of the bidentate ion was much faster than that leading to the simple CO_3^{2-} ion.

Parkyns [63] also investigated the interaction of CO_2 with γ -alumina by infrared spectroscopy.

Four different adsorbed species have been observed and firm assignments made for three of them. The adsorption at $2346 - 2367 \text{ cm}^{-1}$ was considered to be due to the physically adsorbed CO_2 . The adsorption at $3605, 1640, 1480$ and 1233 cm^{-1} was attributed to the formation of bicarbonate groups, and the 1850 and 1180 cm^{-1} bands to bridge structure chemisorbed CO_2 .

In the present study, the bands at $2365, 1800, 1500$ and 1640 cm^{-1} were found when COS alone was adsorbed on the oxygen pretreated γ -alumina at 510°K as shown by figure 21f. This indicates that CO_2 was formed by reaction of the COS with oxygen on the γ -alumina surface. Evacuation caused the disappearance of the 2365 cm^{-1} band. These results agree with the observations by Parkyns [63] and Gregg and Ramsay [31]. With a COS and SO_2 mixture over γ -alumina at 510°K , the IR bands at $3605, 1500, 1640, 2365 \text{ cm}^{-1}$ characteristic of CO_2 adsorption were found. These were shown as figure 23. Evacuation caused the disappearance of the 2365 cm^{-1} band but left the other bands unchanged. When these spectra of the reaction-treated wafer were compared with the baseline spectrum of γ -alumina, it was found that the intensity

of the 3785 cm^{-1} band corresponding to the most active surface hydroxyl group decreased. Such a phenomenon might be due to the formation of a surface bicarbonate from chemisorbed CO_2 and the surface hydroxyl group.

The chemisorbed CO_2 would not desorb from the surface Lewis-acid site of γ -alumina. Consequently, there would be no surface Lewis-acid site available for physical adsorption of COS which is probably essential for the reaction between COS and SO_2 . The catalyst was thus poisoned.

CHAPTER 7

CONCLUSIONS AND RECOMMENDATIONS

Sodium hydroxide doping of the catalyst seems to have the effect of increasing the catalytic activity for the reaction between H_2S and SO_2 but the actual reason why this is so remains unknown. An explanation that the Al-O-Na group formed from the reaction sodium hydroxide and the surface hydroxyl group of the catalyst attracted the H_2S and SO_2 onto the catalyst surface was offered but could not be demonstrated. Infrared spectroscopic technique is not a very good tool in detecting ionic compounds because these compounds usually have absorption vibration frequencies out of the range of infrared spectrum. The Al-O-Na group may have adsorption vibration frequency higher than that of infrared and hence to understand more about the adsorption of H_2S and SO_2 on the NaOH-doped catalysts so that further improvements on catalytic activity can be achieved, it may be beneficial to use ultra-violet spectrophotometry to study this adsorption phenomenon

since the vibration frequencies of ultra-violet light are higher than those of infrared.

The reaction between COS and SO₂ seemed to take place via the physically adsorbed COS and hydrogen bonded SO₂ on γ -alumina. Carbonyl sulfide appeared to be adsorbed through its sulfur end on the Lewis-acid sites and sulfur dioxide was believed to form hydrogen bonding with the surface hydroxyl group of γ -alumina. The irreversible chemisorption of CO₂, formed from the reaction between COS and SO₂ on the Lewis-acid site of the γ -alumina prevented COS from becoming adsorbed on the catalyst and thus poisoned the catalyst. That is why the reaction between COS and SO₂ proceeded over a fresh charge of γ -alumina over a relatively short period of time and then stopped.

Infrared spectrophotometry appears to have provided informations in studying the reaction between COS and SO₂. More should be done to find out how the atoms of COS and SO₂ rearrange on the catalyst surface to form the product, and why CO₂ is chemisorbed on

γ -alumina. To find a catalyst which will catalyze the reaction between COS and SO_2 and not poisoned by CO_2 , it is beneficial to go through those catalysts which past workers found active towards the reaction between COS and SO_2 as a first step in the literature. Then infrared adsorption study on this catalysts should be carried out to find out the activity of the catalysts towards the reaction between COS and SO_2 . Since the infrared spectroscopic investigations were carried out at room temperature, (i.e. the infrared absorption spectra were taken at room temperature) but the reaction between COS and SO_2 was conducted at 510°K , it is possible that the adsorption phenomena measured by infrared spectrophotometer may not be the same as that taking place under reaction temperature in the present study. Therefore, for more reliable informations, infrared investigations should be carried out at reaction temperature in future studies.

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APPENDIX A

CALIBRATION OF EQUIPMENT

A-I Calibration of Thermocouples

The thermocouples were calibrated by immersing each thermocouple and a mercury thermometer in a stirred temperature-controlled oil bath and noting the readings measured by the Honeywell 24 point Electronik 16 millivolt recorder. The physical arrangement used for obtaining the calibration data has been described^{*} along with the fitting of the calibration data to a linear function using least squares. The results are shown in tables A-1 to A-4.

* McGregor, D.E., PhD thesis, University of Alberta, 1971

TABLE A-1 EQUATIONS OF THERMOCOUPLE CALIBRATION RESULTS

Reactor bed temperature ($^{\circ}\text{K}$)

$$= 5.3155 + 18.0706 \times (\text{signal measured in mv})$$

Reactor wall temperature ($^{\circ}\text{K}$)

$$= 6.6860 + 17.9544 \times (\text{signal measured in mv})$$

TABLE A-2

LEAST SQUARE FIT OF CATALYST BED THERMOCOUPLE CALIBRATION
DATA

X = RECORDER READINGS (MILLIVOLTS)

Y = MEASURED TEMPERATURES (DEG. C)

THE COEFFICIENTS OF THE FIRST ORDER POLYNOMIAL ARE

A0 = 5.31550

A1 = 18.07060

REGENERATED DATA

X MEASURED	Y OBSERVED	Y CALCULATED	PCT ERROR
2.826	55.580	56.187	1.081
5.220	99.000	99.644	0.646
10.622	196.200	197.261	0.538
13.537	249.900	249.937	0.015
16.902	310.500	310.745	0.079

VARIANCE = 0.003697

STANDARD DEVIATION = 0.061739

MAXIMUM PCT ERROR = 1.081700

TABLE A-3

LEAST SQUARE FIT OF REACTOR WALL THERMOCOUPLE CALIBRATION DATA

X = RECORDER READINGS (MILLIVOLTS)
Y = MEASURED TEMPERATURES (DEG. C)

THE COEFFICIENT OF THE FIRST ORDER POLYNOMIAL ARE

A0 = 6.68600

A1 = 17.95440

REGENERATED DATA

X MEASURED	Y OBSERVED	Y CALCULATED	PCT ERROR
2.815	57.054	57.231	0.300
5.230	99.000	100.587	1.578
10.501	194.300	195.225	0.474
13.510	249.200	249.250	0.020
16.977	311.500	311.500	0.000

VARIANCE = 0.001544
STANDARD DEVIATION = 0.039295
MAXIMUM PCT ERROR = 1.577861

TABLE A-4

LEAST SQUARE FIT OF FLUIDIZED BED THERMOCOUPLE CALIBRATION
DATA

X = RECORDER READINGS (MILLIVOLTS)

Y = MEASURED TEMPERATURES (DEG. C)

THE COEFFICIENTS OF THE FIRST ORDER POLYNOMIAL ARE

$$A_0 = 6.36270$$

$$A_1 = 17.98530$$

REGENERATED DATA

X MEASURED	Y OBSERVED	Y CALCULATED	PCT ERROR
2.801	56.208	56.747	0.949
5.181	98.600	99.544	0.949
10.641	197.000	197.744	0.376
13.409	247.500	247.528	0.010
17.000	312.100	312.113	0.000

$$\text{VARIANCE} = 0.000683$$

$$\text{STANDARD DEVIATION} = 0.022193$$

$$\text{MAXIMUM PCT ERROR} = 0.949112$$

A-II Calibration of Feed Pressure Transducer

The pressure of the feed stream which was to be calibrated was measured by a Foxboro 611 AH absolute pressure transducer which had a resolution of one mm Hg. The Foxboro 6430 HF electronic consotrol recorder was used to record the pressure signal. To calibrate the absolute pressure transducer, pure nitrogen was passed through the feed line which was also connected to the absolute pressure transducer and a mercury manometer. The reference absolute pressure for the calibration was recorded by adding barometric pressure to the manometer reading. These data were fitted to a straight line using linear least squares and the results of the fit are given in table A-5.

A-III Calibration of Reactor Pressure Transducer

The Statham PA732TC-50-350 absolute pressure transducer, which was used to measure the reactor pressure, was calibrated with the same technique used for the feed pressure transmitter except that the reactor pressure transducer was calibrated at 510°K. Figure A-1 shows the set up of this calibration. The results of the calibration and the linear least square fit of these data are shown in table A-6.

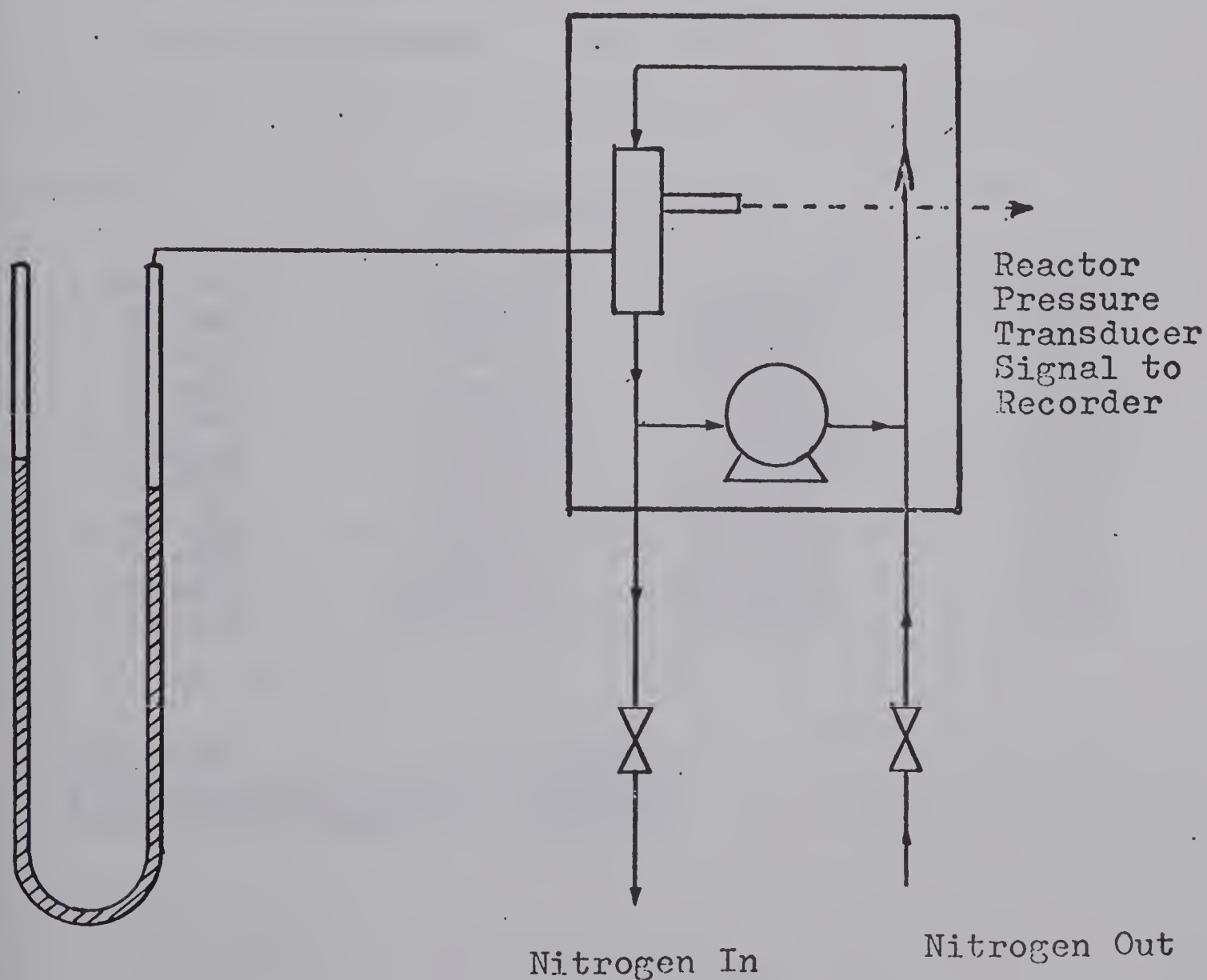


Figure A-1 Calibration of Reactor Pressure Transducer

TABLE A-6

LEAST SQUARE FIT OF REACTOR BED ABSOLUTE PRESSURE
TRANSDUCER CALIBRATION DATA

X = RECORDER READINGS (PERCENT OF FULL SCALE)
Y = ABSOLUTE PRESSURE (MM HG)

THE COEFFICIENT OF THE FIRST ORDER POLYNOMIAL ARE

$$A_0 = -677.57197$$

$$A_1 = 25.91878$$

REGENERATED DATA

X MEASURED	Y OBSERVED	Y CALCULATED	PCT ERROR
53.100	702.000	698.715	0.467
53.400	707.000	706.491	0.071
53.800	716.000	716.858	0.119
54.300	727.500	729.818	0.318
55.900	770.000	771.288	0.167
58.700	844.000	843.860	0.016
61.800	923.000	924.208	0.130
64.300	991.000	989.005	0.201
66.400	1044.000	1043.435	0.054
69.000	1110.000	1110.824	0.074

VARIANCE = 2.808011
STANDARD DEVIATION = 1.675712
MAXIMUM PCT ERROR = 0.467884

A-IV Calibration of Feed Differential Pressure Cell

The feed differential pressure cell was used to measure the flow rate of the feed stream. Pure nitrogen was used to calibrate the differential pressure cell and a density correction was applied when it was used to measure the actual feed stream flow-rate. The density correction was applied in the manner developed by McGregor^{*}. A precalibrated dry test meter (American Meter Company, model number 5M210, serial number 7838179) and a stop watch were used to measure the flow rate of pure nitrogen during calibration. A Foxboro 6430 HF electronic consotrol recorder was used to record the flow rate signal.

The dry test meter was calibrated by passing pure nitrogen through it and then into a five cubic foot gasometer, which had previously been calibrated by filling the bell shape top with water and noting the net weight change with change in height of water. The volume of pure nitrogen passing through the dry test meter and gasometer over the same period of time was noted and the calibration factor was calculated by dividing the volume measured by the dry test meter by that measured by the gasometer. The calibration factors and corresponding

* McGregor, D.E., PhD thesis, University of Alberta, 1971

flow rates were fitted by linear least squares and the results are shown in tables A-7 and A-8. Figure A-2 shows the set up of this calibration.

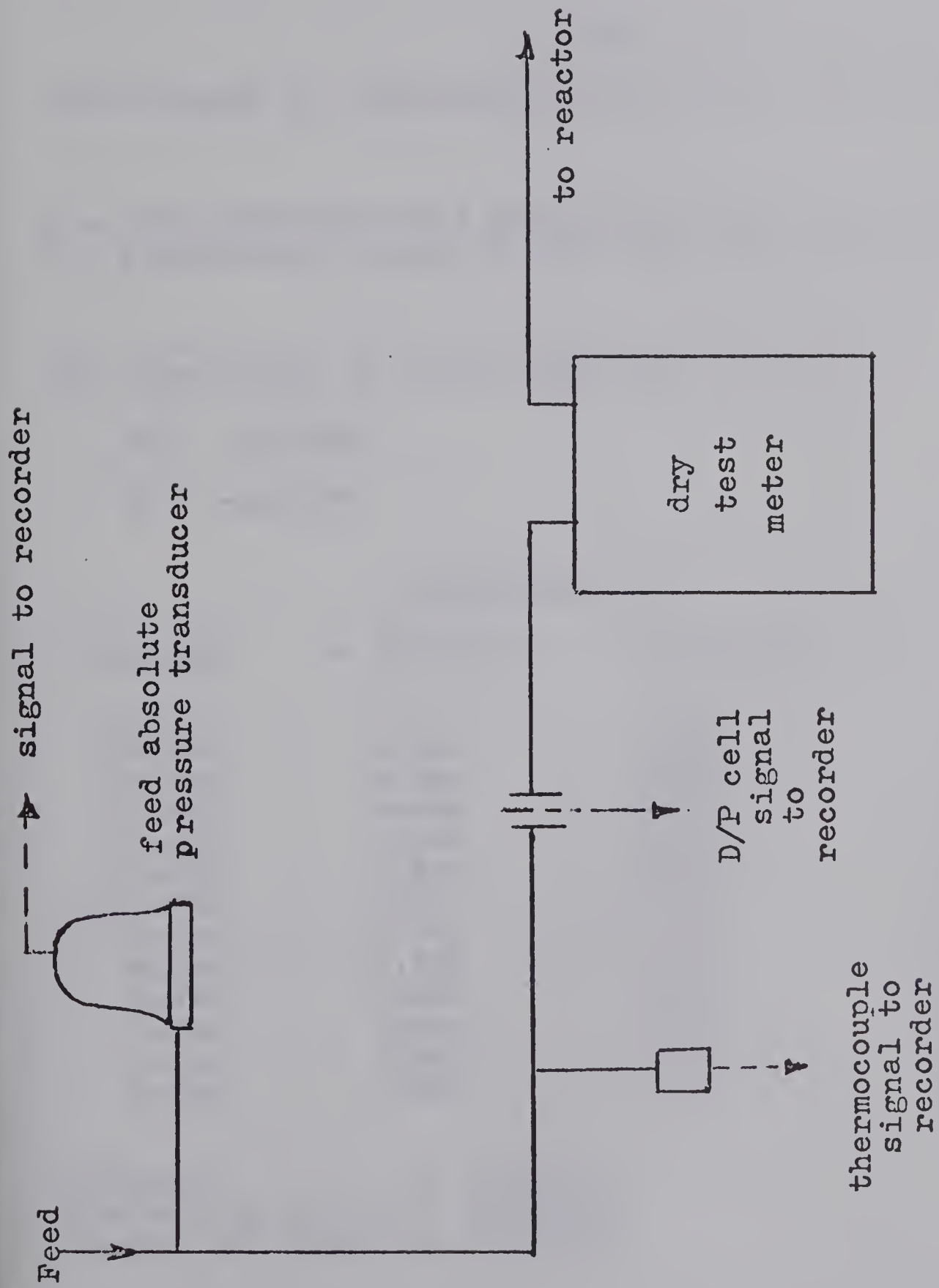


Figure A-2 Differential Pressure Cell Calibration Equipment

TABLE A-7

LEAST SQUARE FIT CALIBRATION FACTOR DATA FOR DRY TEST METER

X = TIME REQUIRED FOR 1 CU. FT. OF GAS FLOW (MIN.)

Y = CALIBRATION FACTOR OF WET TEST METER AGAINST GASOMETER

THE COEFFICIENT OF FIRST ORDER POLYNOMIAL ARE

$$A_0 = 0.99992$$

$$A_1 = -0.00195$$

REGENERATED DATA

X MEASURED	Y OBSERVED	Y CALCULATED	PCT ERROR
19.5			
19.250	0.962	0.962	0.008
18.570	0.963	0.963	0.027
17.060	0.966	0.966	0.042
15.345	0.969	0.969	0.000
13.270	0.973	0.973	0.027
11.730	0.977	0.976	0.052
9.900	0.980	0.980	0.004
9.190	0.982	0.981	0.008
8.200	0.983	0.983	0.035
7.840	0.984	0.984	0.029
7.165	0.985	0.985	0.009
6.700	0.987	0.986	0.051

VARIANCE = 0.000000
 STANDARD DEVIATION = 0.000309
 MAXIMUM PCT ERROR = 0.052002

TABLE A-8

LEAST SQUARE FIT OF FEED D/P CELL DATA AT 24.0 PSIA

X = FOXBORO CHART READING (SQRT(PCT))

Y = FLOW RATE (SCFH)

THE COEFFICIENT OF SECOND ORDER POLYNOMIAL

A0 = 0.91140

A1 = 1.67467

A2 = 0.02285

REGENERATED DATA

X MEASURED	Y OBSERVED	Y CALCULATED	PCT ERROR
1.732	3.879	3.880	0.039
3.162	6.442	6.435	0.104
4.488	8.908	8.887	0.227
5.581	10.919	10.969	0.464
7.059	13.878	13.871	0.044
8.545	16.949	16.890	0.345
9.377	18.585	18.624	0.212
VARIANCE	=	0.001343	
STANDARD DEVIATION	=	0.036658	
MAXIMUM PCT ERROR	=	0.464233	

A-V Calibration of Gas Chromatograph

A five-litre capacity Lucite cylinder equipped with a circulation fan and movable Lucite piston was used for preparing gas mixtures of known composition for calibrations. Lucite, stainless steel 316 and teflon all exhibited inertness toward N_2 , diluted H_2S , COS and SO_2 in this equipment. The fan was driven by a magnetic-coupled motor. The magnet on the process side of the cylinder was coated with a spray-on form of teflon.

To prepare a known composition mixture, pure nitrogen was used to purge the Lucite cylinder and then a measured volume of nitrogen was introduced into the cylinder at atmosphere pressure and room temperature. Then measured volume of other gases could be introduced into the cylinder to mix with nitrogen to give the required composition. Detailed description of the equipment as well as the procedure in preparing a gas mixture had been presented by McGregor*.

The calibration data were reduced by a computer program so that they could be more conveniently fitted by a linear least squares. Since two types of gas mixture involving different components were used in the present studies, two computer program were used. Only the one which involved the COS system will be presented here. The other one had been described in detail by McGregor*.

Results shown in tables A-9 and A-10 are those for the $\text{H}_2\text{S}/\text{SO}_2$ system and tables A-11 to A-16 represent the results of the COS/SO_2 system.

* McGregor, D.E., PhD thesis, University of Alberta, Edmonton, Alberta, 1971

MAINLINE LIU01

ON-LINE GC MONITORING PROGRAM

```

C *****
C *
C *          LIU01
C *
C *  LIU01 IS CALLED  UPON BY PUSH BUTTONS IN THE
C *  LABORATORY TO CARRY OUT ON-LINE GC MONITORING
C *  IT QUEUES LIU02 TO EXECUTE THE GC PEAK DETECTION
C *  AND AREA INTEGRATION
C *
C *****

```

```

EXTERNAL LIU02

```

```

DIMENSION LPID(2),LPHEX(2),IDUM(7)

```

```

DATA LPID/0109,0119/

```

```

DATA LPHEX/Z0109,Z0119/

```

```

DATA IDUM/7*0/

```

```

DEFINE FILE 81(1,1,U,KBS)

```

```

DEFINE FILE 85 (30,7,U,ILU)

```

```

INIT=2

```

```

LUN=9

```

```

  N1,N2,N3 HAVE THE VALUE OF 2 WHEN BUTTON SWITCH IS ON
  AND HAVE THE VALUE OF 1 WHEN BUTTON SWITCH IS OFF

```

```

CALL BTNSW(0,N1)

```

```

CALL BTNSW(1,N2)

```

```

CALL BTNSW(2,N3)

```

```

  FIND THE CONFIGURATION OF THE BUTTON SWITCHES

```

```

N=4*(N1-1)+2*(N2-1)+N3

```

```

GO TO (1,2,3,4,5,6,7,8),N

```

```

  REQUIRED TO TAKE THE GC DATA FOR FEED

```

```

1 CONTINUE

```

```

READ (85'1) ICOUN,IFLAG

```

```

IFLAG=1

```

```

IBS=0

```

```

GO TO 10

```

```

  REQUIRED TO TAKE GC DATA FOR PRODUCT

```

```

2 CONTINUE

```

```

READ (85'1) ICOUN,IFLAG

```

```

IFLAG=2

```

```

IBS=0

```

```

GO TO 10

```

```

  REQUIRED TO PRINT OUT THE THERMAL CONDUCTIVITY CELL
  DIGITAL DATA ONLY

```


MAINLINE LIU01(CONTINUED)

```

4  CONTINUE
   IBS=1
   GO TO 55
C   REQUIRED TO PROCESS THE GC DATA
10  CONTINUE
   WRITE (85'1) ICOUN,IFLAG
55  CONTINUE
   WRITE (81'1) IBS
   CALL QUEUE (LIU02,5,0)
   GO TO 9
C   *** ZERO THE GC FILE
8   DO 20 I=1,30
20  WRITE (85'1) (IDUM(J),J=1,7)
   WRITE (85'1) INIT,INIT
   WRITE (LUN,54)
54  FORMAT (/ ,5X, '**** GC FILE INITIALIZED ****')
   GO TO 9
C   REQUIRED TO TURN ON GC AND TO TAKE GC DATA
C   TURN ECO ON
6   CALL DOUT1 (10,9,1)
   CALL TIME (IHR,IMIN,ISEC)
C   ZERO ACCUMULATION LOOP RECORD
   CALL RSLP (LPHEX(2),K)
C   TURN ON ACQUISITION AND ACCUMULATION LOOP RECORDS
   DO 11 I=1,2
11  CALL OPER (LPID(I))
12  CALL TIME (JHR,JMIN,JSEC)
   ITIME=3600*(JHR-IHR)+60*(JMIN-IMIN)+JSEC-ISEC
   IF (15-ITIME) 13,13,12
C   TURN ECO OFF AFTER IT HAS BEEN TURNED ON FOR 15 SEC
13  CALL DOUT1 (10,9,0)
   WRITE (LUN,51)
51  FORMAT (/ ,10X, '*** GC NOW BEING SCANNED ***' ///)
   IBS=0
   WRITE (81'1) IBS
3   CONTINUE
5   CONTINUE
7   CONTINUE
9   CONTINUE
   WRITE (LUN,52) N
52  FORMAT (10X, '*** CHROMATOGRAM LABBELLED',I4, '***' ///)
   CALL RESET
   CALL VIAQ
   END

```


MAINLINE LIU02

```

C *****
C *
C *                               LIU02                               *
C *
C * LIU02 IS A DISK RESIDENT PROCESS CORELOAD WHICH IS
C * QUEUED BY COMMAND FROM LIU01. ITS PURPOSE IS TO
C * SUPERVISE THE GAS CHROMATOGRAPH PEAK AREA DETECTION*
C * AND DETERMINATION SUBROUTINES. THE PEAK AREAS ARE *
C * TRANSFERRED TO DISK FILE 81 FROM WHICH THEY ARE
C * LATER RECOVERED BY DM001 FOR KINETIC DATA PROCESS- *
C * ING AND REDUCTION.
C *
C *****

```

```

INTEGER RECSZ,DKIN,DKOUT,ERR1,ERR2
DIMENSION LPID(2),LPHEX(2),IDATA(500),START(5),END(5),

```

```
1 ARA(5)
```

```

DEFINE FILE 81 (1,1,U,KBS)
DEFINE FILE 83(64,320,U,IDO)
DEFINE FILE 84(2,320,U,JDO)
DEFINE FILE 85 (30,7,U,ILU)
DATA LPHEX/Z0109,Z0119/
DATA LPID/0109,0119/
DATA END /65.,120.,180.,380.,0./
DATA START/13.,69.,115.,190.,0./
INIT=2
LPDI=LPHEX(2)
NOPTS=400
RECSZ=320
NRECS=2
DKIN=83
DKOUT=84
LUN=9

```

```

C   TURN ACQUISITION AND ACCUMULATION LOOP RECORDS OFF

```

```
CALL NONOP(LPID(2))
```

```
CALL NONOP(LPID(1))
```

```

C   EXTRACT DATA FROM BUFFER USING GBDAT

```

```
CALL NIGBD (LPDI,NOPTS,RECSZ,NRECS,DKIN,DKOUT,NTIME,ER
WRITE (LUN,23) ERR1,ERR2
```

```
23 FORMAT (20X,'ERR1 =',I6/20X,'ERR2 =',I6/////)
```

```

C   ZERO ACCUMULATION RECORD

```

```
CALL RSLP(LPHEX(2),K)
```

```
IF (ERR2-10) 2,2,7.
```

```
2 WRITE (LUN,3)
```

```
3 FORMAT (10X,'***** NUMBER OF DATA LESS THAN 10 **
```

```
GO TO 8
```


MAINLINE LIU02(CONTINUED)

```
7  CONTINUE
   READ(84'1) (IDATA(J),J=1,320)
   READ(84'2) (IDATA(J),J=321,450)
   READ (81'1) IBS
   IF (IBS-1) 10,5,5
10  NUMBR=4
   CALL PKARA (START,END,IDATA,NOPTS,NUMBR,ARA,IBS)
   READ (85'1) ICOUN,IFLAG
   WRITE(85'1) ICOUN,IFLAG,(ARA(J),J=1,4)
   ICOUN=ICOUN+1
   WRITE(85'1) ICOUN,IFLAG
   GO TO 8
5  CONTINUE
   WRITE (LUN,6) (IDATA(J),J=1,391,10)
6  FORMAT (5(2X,8I9/))
8  CONTINUE
   CALL VIAQ
   END
```


SUBROUTINE PKARA

```

C *****
C *
C *          PKARA
C *
C * PKARA CALCULATES THE AREAS OF THE PEAKS
C * WHICH WERE DETECTED BY PKFND.  SIMPSONS RULE
C * INTEGRATION IS USED TO CALCULATE THE AREAS.
C *
C *****
SUBROUTINE PKARA (START,END,Y,NPTS,NUMBR,ARA,IBS)
  INTEGER Y(1)
  DIMENSION AREA(5),START(1),END(1),BCARA(5),ARA(5),
1SNAM(4)
  COMMON IEND(5),NPEAK,ISTRT(5),NAPEX(5),BSAR(5)
  DATA SNAM/'N2  ','CO2 ','COS ','SO2 '/
  H=1.
  LUN=9
  NPEAK=0
  CALL PKFND (Y,NPTS,NCOND)
C  IS THERE ANY PEAK FOUND BY SUBROUTINE LIUPK
  IF (NPEAK) 250,250,1
C  NO PEAK WERE FOUND
250 WRITE(LUN,251) NPEAK
251 FORMAT(5X,'** NO PEAKS FOUND IN DATA, NPEAK=',I5,
1' **'///)
  GO TO 8
1 CONTINUE
  IF (NCOND) 33,33,34
C  END OF DATA DURING PEAK ELUTION
34 WRITE (LUN,35)
35 FORMAT (15X,'*-*-* END OF DATA DURING PEAK ELUTION
1*-*-* '///)
33 CONTINUE
C  SOME PEAKS HAD BEEN FOUND
  WRITE (LUN,32) NPEAK
32 FORMAT (10X,'NUMBER OF PEAKS FOUND IS =',I6///)
  WRITE (LUN,31)
31 FORMAT (10X,'COMPONENT  PK START      PK END      PK ',
1'AREA'/
110X,'-----  -----  -----  -----'///)
  DO 120 K=1,NPEAK
  AREA(K)=0.
C  APEX IS REQUIRED FOR 1ST AND 2ND PEAKS
  IF (IBS-3) 3,3,2
3 CONTINUE

```


SUBROUTINE PKARA.....(CONTINUED)

```

      IF (K-2) 4,4,5
2    IF (K-1) 4,4,5
5    L=IEND(K)-ISTRT(K)
      IAPFL=3
      AR1=0.
      X=FLOAT(L)/2.
      L=L/2
C    CHECK NO. OF INTERVALS EVEN OR ODD
      IF (X-L) 22,22,21
C    ODD NUMBER OF INTERVALS      ADD ONE INTERVAL TO PEAK
21   IEND(K)=IEND(K)+1
22   IBGN=ISTRT(K)+1
      JEND=IEND(K)-1
      GO TO 20
4    ISTR=ISTRT(K)
      L=IEND(K)-ISTRT(K)
      CALL APEX (L,Y,APARA,ISTR,IFL,IBF)
      L=IFL-ISTRT(K)
      IAPFL=0
      JEND=IFL
      IBGN=ISTRT(K)
      GO TO 6
16   L=IEND(K)-IBF
      IBGN=IBF
      JEND=IEND(K)
C    CHECK IF NUMBER INTERVALS EVEN OR ODD
6    X=FLOAT(L)/2.
      L=L/2
      IF (X-L) 20,20,10
C    ODD NUMBER OF INTERVALS ADD ONE INTERVAL TO PEAK
10   IF (IAPFL) 12,12,11
11   JEND=IEND(K)-1
      GO TO 20
12   IBGN=ISTRT(K)+1
C    SIMPSONS RULE INTEGRATION
20   JJEND=JEND-2
      DO 40 I=IBGN,JJEND,2
40   AREA(K)=AREA(K)+Y(I)+4.*Y(I+1)+Y(I+2)
      AREA(K)=AREA(K)*H/3.
      IF (K-2) 126,126,127
126  CONTINUE
      IF (IAPFL) 14,14,15
14   CONTINUE
      AR1=AREA(K)
      AREA(K)=0.

```


SUBROUTINE PKARA.....(CONTINUED)

```

      IAPFL=1
      GO TO 16
15  CONTINUE
      AR2=AREA(K)
      AR3=AR1+AR2+APARA
C    BASE-LINE CORRECTED AREA
      BCARA(K)=AR3-BSAR(K)
      CONST=BCARA(K)/FLOAT(NAPEX(K))
      GO TO 80
127 CONTINUE
C    BASE-LINE CORRECTED AREA
      BCARA(K)=AREA(K)-BSAR(K)
      CONST=BCARA(K)/FLOAT(NAPEX(K))
80  CONTINUE
      IF (NPEAK-3) 81,82,82
81  IF (K-1) 82,82,83
82  KSPCD=K
      GO TO 84
83  IF (IBS-0) 8,70,71
70  KSPCD=K
      GO TO 84
71  KSPCD=IBS
84  CONTINUE
      WRITE (LUN,85) SNAM(KSPCD),ISTRRT(K),IEND(K),BCARA(K)
85  FORMAT (12X,A4,5X,I6,4X,I6,4X,F13.2/)
120 CONTINUE
C    CHECK IF NO. OF PEAKS FOUND = NO. SPECIFIED
      IF (NUMBR-NPEAK) 122,125,122
122 CONTINUE
      WRITE (LUN,90)
90  FORMAT (15X,'*-*-* NUMBER OF PEAKS FOUND DIFF. FROM',
1' SPECIFIED *-*-*'////////)
125 CONTINUE
8   CONTINUE
      RETURN
      END

```


SUBROUTINE PKFND

```

C *****
C *
C *          PKFND
C *
C * PKFND DETERMINES PEAK EVENTS BY EXAMINATION OF THE
C * FIRST DERIVATIVE OF THE THERMAL CONDUCTIVITY
C * DETECTOR SIGNAL. PERTINENT DATA IS TRANSFERRED
C * BACK TO PKARA FOR CALCULATION OF PEAK AREAS.
C *
C *****
SUBROUTINE PKFND (Y,NPTS,NCOND)
  INTEGER Y(1)
  DIMENSION NEN(5),NST(5)
  COMMON IEND(5),NPEAK,ISTRT(5),NAPEX(5),BSAR(5)
  DATA DBST,DBEND,ITEST/3.0,3.0,3/
  DATA DRV1,DRV1A,ICFST,ICFED,NGHG/0.,0.,0,0,0/
  NPEAK=0
  H=1.
  NCOND=0
  LUN=9
  BSAR(1)=0.
  BSAR(2)=0.
  BSAR(3)=0.
  BSAR(4)=0.
  BSAR(5)=0.
  NDATA=NPTS-4
  DO 200 I=3,NDATA
    DRV1B=DRV1
C    COMPUTE FIRST DERIVATIVE AT Y(I)
    DRV1=DRV1A
C    COMPUTE FIRST DERIVATIVE AT Y(I+1)
C    SEVEN POINT LEAST SQUARES ESTIMATE OF FIRST DERIVATIVE
    DRV1A=3.*(Y(I+4)-Y(I-2))+2.*(Y(I+3)-Y(I-1))+
1Y(I+2)-Y(I)
    DRV1A=DRV1A/(28.*H)
C    IS PEAK IN PROGRESS
    IF(NCOND)10,10,40
C    PEAK IS NOT PROGRESS
C    CHECK FIRST DERIVATIVE FOR PEAK START
10  IF(DRV1-DBST) 200,20,20
C    CONFIRM PEAK START ITEST TIMES
20  ICFST=ICFST+1
25  IF(ICFST-ITEST)200,30,30
C    PEAK HAS STARTED
30  NCOND=1

```


SUBROUTINE PKFND.....(CONTINUED)

```

C      INCREMENT PEAK COUNTER
      NPEAK=NPEAK+1
      IF (NPEAK-5) 300,300,301
300  CONTINUE
C      SAVE INDEX OF STARTING POINT
      ISTRT(NPEAK)=I-ITEST+1
      IIST=ISTRT(NPEAK)
      NST(NPEAK)=Y(IIST)
      ICFST=0
      GO TO 200
C      CHECK FOR PEAK END
C      HAS FIRST DERIVATIVE GONE +VE TO -VE
40  IF(NGHG)50,50,70
50  IF(DRV1)60,200,200
C      FIRST DERIVATIVE HAS GONE +VE TO -VE
60  NGHG=1
C      SAVE INDEX OF PEAK HEIGHT
      IF (Y(I)-Y(I-1)) 41,45,45
41  NAPEX(NPEAK)=Y(I-1)
      IMAX=I-1
      GO TO 70
45  NAPEX(NPEAK)=Y(I)
      IMAX=I
C      CHECK FOR PEAK END
70  IF(DRV1+DBEND)200,80,80
C      CONFIRM PEAK END
80  ICFED=ICFED+1
C      CHECK FOR START OF NEW PEAK
      IF(DRV1-DBST)77,75,75
75  ICFST=ICFST+1
      GO TO 78
77  ICFST=0
78  IF(ICFED-ITEST)200,87,87
C      PEAK END
C      SAVE INDEX OF END POINT
87  IEND(NPEAK)=I
      NEN(NPEAK)=Y(I)
      NFRNT=NAPEX(NPEAK)-NST(NPEAK)
      NBK=NAPEX(NPEAK)-NEN(NPEAK)
      L=IEND(NPEAK)-ISTRT(NPEAK)
C      CHECK IF THE DETECTED PEAK IS NOISE
      IF (L-10) 33,33,22
33  NPEAK=NPEAK-1
      GO TO 37
22  CONTINUE

```


SUBROUTINE PKFND.....(CONTINUED)

```

C      CHECK IF THE DETECTED PEAK IS BASELINE DRIFT
      IF (NFRNT-500) 31,31,38
38     IF (NBK-500) 31,31,35
C      YES      DECREASE PEAK COUNTER
31     NPEAK=NPEAK-1
      GO TO 37
35     CONTINUE
      IF (NPEAK) 202,202,201
201    CONTINUE
      BSAR(NPEAK)=(FLOAT(NEN(NPEAK)+NST(NPEAK)))*
      1(FLOAT(IEND(NPEAK)-ISTRT(NPEAK)))/2.
C      CHECK FOR IMMEDIATE START OF NEW PEAK
37     CONTINUE
      IF(ICFST)88,88,25
88     ICFED=0
      NCOND=0
      NGHG=0
      ICFST=0
200    CONTINUE
      GO TO 400
202    CONTINUE
      WRITE (LUN,203)
203    FORMAT (10X,'***** NPEAK=0 *****'///)
      GO TO 400
301    CONTINUE
      WRITE (LUN,302) NPEAK
302    FORMAT (10X,'NPEAK =',I5///)
400    CONTINUE
      RETURN
      END

```


SUBROUTINE APEX

```

*****
*
*                               APEX
*
* APEX IS USED TO ANALYTICALLY CALCULATE THE AREA OF
* THE APEX OF SHARP PEAKS.
*
*****

```

```

SUBROUTINE APEX (NPTS,Y,APARA,ISTR,IFL,IBF)
  INTEGER Y(1)
  DIMENSION SM(8),X(11)
  DATA X/0.,1.,2.,3.,4.,5.,6.,7.,8.,9.,10./
  DO 20 I=1,8
20 SM(I)=0.
  M=3
  ISTR=ISTR+1
  NPT=NPTS+ISTR
  DO 1 I=ISTR,NPT
  DER2=Y(I)-Y(I-1)
  DER3=Y(I+1)-Y(I)
  IF (DER3) 1,1,2
2 IF (DER3-DER2) 3,3,1
3 DER4=Y(I+2)-Y(I+1)
  IF (DER4) 5,1,1
5 IF (DER4+DER2-2.*DER3) 6,6,7
6 IBF=I+1
  IFL=I
  GO TO 8
7 IFL=I+1
  IBF=I+2
  GO TO 8
1 CONTINUE
8 DO 9 I=1,M
  J=I+M
  J1=IFL-I+1
  J2=IFL-M+I
  J3=IBF+I-1
  SM(1)=SM(1)+X(I)
  SM(2)=SM(2)+Y(J1)
  SM(3)=SM(3)+X(I)*Y(J2)
  SM(4)=SM(4)+X(J)
  SM(5)=SM(5)+Y(J3)
  SM(6)=SM(6)+X(J)*Y(J3)
  SM(7)=SM(7)+X(I)**2
  SM(8)=SM(8)+X(J)**2

```


SUBROUTINE APEX(CONTINUED)

9 CONTINUE

A1F=(M*SM(3)-SM(1)*SM(2))/(M*SM(7)-SM(1)**2)

A1B=(M*SM(6)-SM(4)*SM(5))/(M*SM(8)-SM(4)**2)

A0F=(SM(7)*SM(2)-SM(3)*SM(1))/(M*SM(7)-SM(1)**2)

A0B=(SM(8)*SM(5)-SM(6)*SM(4))/(M*SM(8)-SM(4)**2)

APARA=(A0F-A0B)**2/(2.*(A1B-A1F))-X(M)*(A0F+X(M)*A1F
1/2.)+X(M+1)*(A0B+X(M+1)*A1B/2.)

RETURN

END

MAINLINE GCCOS(CONTINUED)

RTEM=(RTEM+460.)/1.8
BTEM=(BTEM+460.)/1.8

C
C
C
CALCULATION OF SAMPLE COMPOSITION

XMN2=(11.+151.192*V(1))*STEMP/RTEM*APRES/SPRES/SMV(1)
V(1)=(11.+151.192*V(1))
XMCAL=V(2)*STEMP/BTEM*APRES/SPRES/SMV(IPEAK)
TOTM=XMN2+XMCAL
XMN2=XMN2/TOTM*100.
XMCAL=XMCAL/TOTM*100.
RMOL=XMCAL/XMN2*100.
KPEAK=IPEAK-1

C
C
C
READ AND PROCESS PEAK AREA DATA

NCAT=0
14 DO 4 I=1,7
4 AVG(I)=0.0
DO 5 ICROM=1,NCROM
NCAT=NCAT+1
READ(5,3) RDG
RDG(5)=RDG(2)*(21.-2.*RDG(4))
RDG(4)=RDG(2)
RDG(2)=RDG(1)*(21.-2.*RDG(3))
TOTA=RDG(2)+RDG(5)
RDG(3)=RDG(2)/TOTA*100.
RDG(6)=RDG(5)/TOTA*100.
RDG(7)=RDG(5)/RDG(2)*100.
DO 6 I=1,7
6 AVG(I)=RDG(I)+AVG(I)
DO 20 J=1,7
20 STORE(NCAT,J)=RDG(J)
5 CONTINUE
DO 7 I=1,7
7 AVG(I)=AVG(I)/NCROM
NCAT=NCAT+1
DO 21 J=1,7
21 STORE(NCAT,J)=AVG(J)
IF(ICOMP) 9,9,8
8 ICOMP=0
GO TO 14
9 CONTINUE
NN=NCROM+1
N1=NN+1

MAINLINE GCCOS

```

C *****
C *
C *          MAINLINE GCCOS
C *
C * THIS PROGRAM WAS WRITTEN TO DOCUMENT THE DATA
C * TAKEN FOR THE CALIBRATION OF THE PROCESS GAS
C * CHROMATOGRAPH AND REDUCE THIS DATA TO CALCULATED
C * RESULTS USEFUL FOR THE INTERNAL STANDARD PROCEDURE
C * FOR THE CALIBRATION OF GAS CHROMATOGRAPHS.
C *   INPUT DATA
C *       NSET   - NUMBER OF SETS OF DATA
C *       NCOPY  - NUMBER OF COPIES OF OUTPUT DESIRED
C *       NPAGE  - PAGE NUMBER OF FIRST PAGE OF OUTPUT
C *       NRUN   - CALIBRATION RUN NUMBER
C *       NCROM  - NUMBER OF CHROMATOGRAMS TAKEN
C *       IPEAK  - PEAK NUMBER CALIBRATED
C *               ...2 - CO2
C *               ...3 - COS
C *               ...4 - SO2
C *       ICOMP  - AREA FLAG
C *               ...1 - COMPUTER AREAS INCLUDED
C *               ...0 - NO COMPUTER AREAS
C *       RTEM   - ROOM TEMPERATURE (DEG F)
C *       APRES  - ATMOSPHERIC PRESSURE (MM HG)
C *       BTEM   - WATER BATH TEMPERATURE (DEG F)
C *       V(1)   - DISTANCE BETWEEN PISTON AND END OF
C *               CYLINDER (CM)
C *       V(2)   - VOLUME OF CALIBRATION GAS (CU CM)
C *       RDG(1) - AREA OF NITROGEN PEAK
C *       RDG(2) - AREA OF CALIBRATION GAS
C *       RDG(3) - ATTENUATION FOR NITROGEN
C *       RDG(4) - ATTENUATION FOR CALIBRATION GAS
C *****
C   DIMENSION SNAM(4,3),SMV(4),V(2),RDG(7),AVG(7),
C 1STORE(20,7)
C   DATA SMV/22403.60,22346.10,22399.54,21889.30/
C   DATA SNAM/'CARB','ON D','IOXI','DE  ','CARB','ONYL','
C 1,'SULF','UR D','IOXI','DE  '/
C   READ(5,1) NSET,NCOPY,NPAGE
C   DO 2 ISET=1,NSET
C   READ(5,1) NRUN,NCROM,IPEAK,ICOMP
C   READ(5,3) RTEM,BTEM,APRES,V(1),V(2)
C   STEMP=273.
C   SPRES=760.

```


MAINLINE GCCOS(CONTINUED)

```

N2=2*NN
DO 23 IC=1,NCOPY
WRITE(6,17) NPAGE
WRITE(6,10) NRUN,RTEM,BTEM
WRITE (6,30) APRES,V(1),(SNAM(J,KPEAK),J=1,4),V(2)
WRITE(6,11) XMN2,(SNAM(J,KPEAK),J=1,4),XMCAL,RMOL
WRITE(6,12)
WRITE(6,13) (SNAM(J,KPEAK),J=1,4)
WRITE(6,15) ((STORE(I,J),J=1,7),I=1,NN)
WRITE(6,16)
WRITE(6,15) ((STORE(I,J),J=1,7),I=N1,N2)
23 CONTINUE
NPAGE=NPAGE+1
2 CONTINUE
1 FORMAT(5I5)
3 FORMAT (7F10.2)
10 FORMAT(      15X,'CALIBRATION SAMPLE NUMBER',I3,///10X,
1'SAMPLE PREPARATION CONDITIONS'//12X,
2'ROOM TEMPERATURE.....',F7.1,
3' DEG K',//12X,'BATH TEMPERATURE.....',F7.1,
4' DEG K',//)
30 FORMAT (12X,'ATMOSPHERIC PRESSURE.....',F7.1,' MM HG'
1,//12X,'VOLUME OF NITROGEN.....',F7.1,' CC',//12X,
2'VOLUME OF ',4A4,F7.1,' CC')
11 FORMAT( //,10X,'SAMPLE COMPOSITION (MOLE PERCENT)'//
112X,'NITROGEN.....',F6.2,//12X,4A4,'...',F6.2,//
212X,'100X MOLAR RATIO...',F6.2)
12 FORMAT( //,10X,'DISK INTEGRATOR AREA RESULTS (THE ',
1'LAST SET IS THE AVERAGE)'//)
13 FORMAT (17X,'NITROGEN',18X,4A4, 8X,'100X',//9X,'INPUT'
1,5X,'CORR',4X,'PCT OF',7X,'INPUT',4X,'CORR',5X,
2'PCT OF',3X,'AREA' / 9X,'AREA',6X,'AREA',4X,'TOTAL',8X
3,'AREA',5X,'AREA',5X,'TOTAL',4X,'RATIO'//)
15 FORMAT (6X,F8.1,1X,F9.1,2X,F6.2,5X,F8.1,1X,F8.1,2X,
1F6.2,3X,F6.2//)
16 FORMAT( /,10X,'COMPUTER AREA RESULTS (THE LAST SET ',
1'IS THE AVERAGE)'//)
17 FORMAT('1',///66X,'A-',I2,//)
CALL EXIT
END

```


H2S/SO2 SYSTEM

CALIBRATION SAMPLE NUMBER 1

SAMPLE PREPARATION CONDITIONS

ROOM TEMPERATURE..... 295.0 DEG K

BATH TEMPERATURE..... 293.8 DEG K

ATMOSPHERIC PRESSURE..... 703.1 MM HG

VOLUME OF NITROGEN..... 4619.3 CC

VOLUME OF SULFUR DIOXIDE 26.2 CC

SAMPLE COMPOSITION (MOLE PERCENT)

NITROGEN..... 99.42

SULFUR DIOXIDE ... 0.57

100X MOLAR RATIO... 0.58

DISK INTEGRATOR AREA RESULTS (THE LAST SET IS THE AVERAGE)

NITROGEN			SULFUR DIOXIDE			100X
INPUT AREA	CORR AREA	PCT OF TOTAL	INPUT AREA	CORR AREA	PCT OF TOTAL	AREA RATIO
85.5	3676.5	98.71	60.0	48.0	1.28	1.30
83.0	3652.0	98.71	59.4	47.5	1.28	1.30
84.2	3664.2	98.71	59.7	47.7	1.28	1.30

COMPUTER AREA RESULTS (THE LAST SET IS THE AVERAGE)

0.0	0.0	0.00	0.0	0.0	0.00	0.00
0.0	0.0	0.00	0.0	0.0	0.00	0.00
0.0	0.0	0.00	0.0	0.0	0.00	0.00

H2S/SO2 SYSTEM

CALIBRATION SAMPLE NUMBER 2

SAMPLE PREPARATION CONDITIONS

ROOM TEMPERATURE..... 293.3 DEG K
BATH TEMPERATURE..... 293.3 DEG K
ATMOSPHERIC PRESSURE..... 703.1 MM HG
VOLUME OF NITROGEN..... 4619.3 CC
VOLUME OF SULFUR DIOXIDE 53.7 CC

SAMPLE COMPOSITION (MOLE PERCENT)

NITROGEN..... 98.82
SULFUR DIOXIDE ... 1.17
100X MOLAR RATIO... 1.18

DISK INTEGRATOR AREA RESULTS (THE LAST SET IS THE AVERAGE)

NITROGEN			SULFUR DIOXIDE			100X
INPUT AREA	CORR AREA	PCT OF TOTAL	INPUT AREA	CORR AREA	PCT OF TOTAL	AREA RATIO
82.7	3638.8	97.40	121.0	96.8	2.59	2.66
82.8	3643.1	97.40	121.4	97.1	2.59	2.66
82.7	3640.9	97.40	121.2	96.9	2.59	2.66

COMPUTER AREA RESULTS (THE LAST SET IS THE AVERAGE)

0.0	0.0	0.00	0.0	0.0	0.00	0.00
0.0	0.0	0.00	0.0	0.0	0.00	0.00
0.0	0.0	0.00	0.0	0.0	0.00	0.00

H₂S/SO₂ SYSTEM

CALIBRATION SAMPLE NUMBER 3

SAMPLE PREPARATION CONDITIONS

ROOM TEMPERATURE..... 295.5 DEG K
BATH TEMPERATURE..... 294.4 DEG K
ATMOSPHERIC PRESSURE..... 703.1 MM HG
VOLUME OF NITROGEN..... 4619.3 CC
VOLUME OF SULFUR DIOXIDE 73.9 CC

SAMPLE COMPOSITION (MOLE PERCENT)

NITROGEN..... 98.38
SULFUR DIOXIDE ... 1.61
100X MOLAR RATIO... 1.64

DISK INTEGRATOR AREA RESULTS (THE LAST SET IS THE AVERAGE)

NITROGEN			SULFUR DIOXIDE			100X
INPUT AREA	CORR AREA	PCT OF TOTAL	INPUT AREA	CORR AREA	PCT OF TOTAL	AREA RATIO
83.0	3652.0	96.40	170.0	136.0	3.59	3.72
82.5	3630.0	96.42	168.0	134.4	3.57	3.70
82.7	3641.0	96.41	169.0	135.2	3.58	3.71

COMPUTER AREA RESULTS (THE LAST SET IS THE AVERAGE)

0.0	0.0	0.00	0.0	0.0	0.00	0.00
0.0	0.0	0.00	0.0	0.0	0.00	0.00
0.0	0.0	0.00	0.0	0.0	0.00	0.00

H₂S/SO₂ SYSTEM

CALIBRATION SAMPLE NUMBER 4

SAMPLE PREPARATION CONDITIONS

ROOM TEMPERATURE..... 295.5 DEG K

BATH TEMPERATURE..... 294.4 DEG K

ATMOSPHERIC PRESSURE..... 703.1 MM HG

VOLUME OF NITROGEN..... 4619.3 CC

VOLUME OF SULFUR DIOXIDE 83.6 CC

SAMPLE COMPOSITION (MOLE PERCENT)

NITROGEN..... 98.17

SULFUR DIOXIDE ... 1.82

100X MOLAR RATIO... 1.85

DISK INTEGRATOR AREA RESULTS (THE LAST SET IS THE AVERAGE)

NITROGEN			SULFUR DIOXIDE			100X
INPUT AREA	CORR AREA	PCT OF TOTAL	INPUT AREA	CORR AREA	PCT OF TOTAL	AREA RATIO
83.8	3687.1	96.03	190.5	152.4	3.96	4.13
82.5	3630.0	96.03	187.4	149.9	3.96	4.13
83.1	3658.6	96.03	188.9	151.1	3.96	4.13

COMPUTER AREA RESULTS (THE LAST SET IS THE AVERAGE)

0.0	0.0	0.00	0.0	0.0	0.00	0.00
0.0	0.0	0.00	0.0	0.0	0.00	0.00
0.0	0.0	0.00	0.0	0.0	0.00	0.00

H2S/SO2 SYSTEM

CALIBRATION SAMPLE NUMBER 5

SAMPLE PREPARATION CONDITIONS

ROOM TEMPERATURE..... 295.5 DEG K
BATH TEMPERATURE..... 294.4 DEG K
ATMOSPHERIC PRESSURE..... 703.1 MM HG
VOLUME OF NITROGEN..... 4619.3 CC
VOLUME OF SULFUR DIOXIDE 94.9 CC

SAMPLE COMPOSITION (MOLE PERCENT)

NITROGEN..... 97.93
SULFUR DIOXIDE ... 2.06
100X MOLAR RATIO... 2.11

DISK INTEGRATOR AREA RESULTS (THE LAST SET IS THE AVERAGE)

NITROGEN			SULFUR DIOXIDE			100X
INPUT AREA	CORR AREA	PCT OF TOTAL	INPUT AREA	CORR AREA	PCT OF TOTAL	AREA RATIO
82.9	3647.6	95.50	214.8	171.8	4.49	4.71
81.0	3564.0	95.50	209.8	167.8	4.49	4.70
81.9	3605.8	95.50	212.3	169.8	4.49	4.71

COMPUTER AREA RESULTS (THE LAST SET IS THE AVERAGE)

0.0	0.0	0.00	0.0	0.0	0.00	0.00
0.0	0.0	0.00	0.0	0.0	0.00	0.00
0.0	0.0	0.00	0.0	0.0	0.00	0.00

H2S/SO2 SYSTEM

CALIBRATION SAMPLE NUMBER 6

SAMPLE PREPARATION CONDITIONS

ROOM TEMPERATURE..... 293.3 DEG K

BATH TEMPERATURE..... 292.7 DEG K

ATMOSPHERIC PRESSURE..... 703.1 MM HG

VOLUME OF NITROGEN..... 4619.3 CC

VOLUME OF SULFUR DIOXIDE 109.7 CC

SAMPLE COMPOSITION (MOLE PERCENT)

NITROGEN..... 97.62

SULFUR DIOXIDE ... 2.37

100X MOLAR RATIO... 2.43

DISK INTEGRATOR AREA RESULTS (THE LAST SET IS THE AVERAGE)

NITROGEN			SULFUR DIOXIDE			100X
INPUT AREA	CORR AREA	PCT OF TOTAL	INPUT AREA	CORR AREA	PCT OF TOTAL	AREA RATIO
83.5	3674.0	94.73	255.0	204.0	5.26	5.55
84.2	3704.8	94.70	259.1	207.2	5.29	5.59
83.8	3689.4	94.72	257.0	205.6	5.27	5.57

COMPUTER AREA RESULTS (THE LAST SET IS THE AVERAGE)

0.0	0.0	0.00	0.0	0.0	0.00	0.00
0.0	0.0	0.00	0.0	0.0	0.00	0.00
0.0	0.0	0.00	0.0	0.0	0.00	0.00

H₂S/SO₂ SYSTEM

CALIBRATION SAMPLE NUMBER 7

SAMPLE PREPARATION CONDITIONS

ROOM TEMPERATURE..... 293.8 DEG K

BATH TEMPERATURE..... 293.3 DEG K

ATMOSPHERIC PRESSURE..... 703.1 MM HG

VOLUME OF NITROGEN..... 4619.3 CC

VOLUME OF HYDROGEN SULFIDE 51.5 CC

SAMPLE COMPOSITION (MOLE PERCENT)

NITROGEN..... 98.88

HYDROGEN SULFIDE... 1.11

100X MOLAR RATIO... 1.13

DISK INTEGRATOR AREA RESULTS (THE LAST SET IS THE AVERAGE)

NITROGEN			HYDROGEN SULFIDE			100X
INPUT AREA	CORR AREA	PCT OF TOTAL	INPUT AREA	CORR AREA	PCT OF TOTAL	AREA RATIO
85.1	3744.3	97.69	63.0	88.2	2.30	2.35
85.8	3775.1	97.65	64.8	90.7	2.34	2.40
85.4	3759.7	97.67	63.9	89.4	2.32	2.37

COMPUTER AREA RESULTS (THE LAST SET IS THE AVERAGE)

0.0	0.0	0.00	0.0	0.0	0.00	0.00
0.0	0.0	0.00	0.0	0.0	0.00	0.00
0.0	0.0	0.00	0.0	0.0	0.00	0.00

H2S/SO2 SYSTEM

CALIBRATION SAMPLE NUMBER 8

SAMPLE PREPARATION CONDITIONS

ROOM TEMPERATURE..... 293.3 DEG K

BATH TEMPERATURE..... 293.3 DEG K

ATMOSPHERIC PRESSURE..... 703.1 MM HG

VOLUME OF NITROGEN..... 4619.3 CC

VOLUME OF HYDROGEN SULFIDE 87.4 CC

SAMPLE COMPOSITION (MOLE PERCENT)

NITROGEN..... 98.12

HYDROGEN SULFIDE... 1.87

100X MOLAR RATIO... 1.91

DISK INTEGRATOR AREA RESULTS (THE LAST SET IS THE AVERAGE)

NITROGEN			HYDROGEN SULFIDE			100X
INPUT AREA	CORR AREA	PCT OF TOTAL	INPUT AREA	CORR AREA	PCT OF TOTAL	AREA RATIO
83.0	3652.0	96.24	101.9	142.6	3.75	3.90
83.1	3656.3	96.23	102.1	142.9	3.76	3.90
83.0	3654.2	96.23	101.9	142.8	3.76	3.90

COMPUTER AREA RESULTS (THE LAST SET IS THE AVERAGE)

0.0	0.0	0.00	0.0	0.0	0.00	0.00
0.0	0.0	0.00	0.0	0.0	0.00	0.00
0.0	0.0	0.00	0.0	0.0	0.00	0.00

H₂S/SO₂ SYSTEM

CALIBRATION SAMPLE NUMBER 9

SAMPLE PREPARATION CONDITIONS

ROOM TEMPERATURE..... 293.3 DEG K

BATH TEMPERATURE..... 293.3 DEG K

ATMOSPHERIC PRESSURE..... 703.1 MM HG

VOLUME OF NITROGEN..... 4619.3 CC

VOLUME OF HYDROGEN SULFIDE 103.8 CC

SAMPLE COMPOSITION (MOLE PERCENT)

NITROGEN..... 97.77

HYDROGEN SULFIDE... 2.22

100X MOLAR RATIO... 2.27

DISK INTEGRATOR AREA RESULTS (THE LAST SET IS THE AVERAGE)

NITROGEN			HYDROGEN SULFIDE			100X
INPUT AREA	CORR AREA	PCT OF TOTAL	INPUT AREA	CORR AREA	PCT OF TOTAL	AREA RATIO
82.2	3616.8	95.53	120.8	169.1	4.46	4.67
82.5	3630.0	95.55	120.5	168.7	4.44	4.64
82.3	3623.4	95.54	120.6	168.9	4.45	4.66

COMPUTER AREA RESULTS (THE LAST SET IS THE AVERAGE)

0.0	0.0	0.00	0.0	0.0	0.00	0.00
0.0	0.0	0.00	0.0	0.0	0.00	0.00
0.0	0.0	0.00	0.0	0.0	0.00	0.00

H₂S/SO₂ SYSTEM

CALIBRATION SAMPLE NUMBER 10

SAMPLE PREPARATION CONDITIONS

ROOM TEMPERATURE..... 292.7 DEG K
BATH TEMPERATURE..... 292.7 DEG K
ATMOSPHERIC PRESSURE..... 703.1 MM HG
VOLUME OF NITROGEN..... 4619.3 CC
VOLUME OF HYDROGEN SULFIDE 146.3 CC

SAMPLE COMPOSITION (MOLE PERCENT)

NITROGEN..... 96.89
HYDROGEN SULFIDE... 3.10
100X MOLAR RATIO... 3.20

DISK INTEGRATOR AREA RESULTS (THE LAST SET IS THE AVERAGE)

NITROGEN			HYDROGEN SULFIDE			100X
INPUT AREA	CORR AREA	PCT OF TOTAL	INPUT AREA	CORR AREA	PCT OF TOTAL	AREA RATIO
82.5	3630.0	93.76	172.3	241.2	6.23	6.64
82.6	3634.3	93.80	171.5	240.1	6.19	6.60
82.5	3632.2	93.78	171.9	240.6	6.21	6.62

COMPUTER AREA RESULTS (THE LAST SET IS THE AVERAGE)

0.0	0.0	0.00	0.0	0.0	0.00	0.00
0.0	0.0	0.00	0.0	0.0	0.00	0.00
0.0	0.0	0.00	0.0	0.0	0.00	0.00

H₂S/SO₂ SYSTEM

CALIBRATION SAMPLE NUMBER 11

SAMPLE PREPARATION CONDITIONS

ROOM TEMPERATURE..... 293.3 DEG K

BATH TEMPERATURE..... 292.7 DEG K

ATMOSPHERIC PRESSURE..... 703.1 MM HG

VOLUME OF NITROGEN..... 4619.3 CC

VOLUME OF HYDROGEN SULFIDE 170.2 CC

SAMPLE COMPOSITION (MOLE PERCENT)

NITROGEN..... 96.39

HYDROGEN SULFIDE... 3.60

100X MOLAR RATIO... 3.73

DISK INTEGRATOR AREA RESULTS (THE LAST SET IS THE AVERAGE)

NITROGEN			HYDROGEN SULFIDE			100X
INPUT AREA	CORR AREA	PCT OF TOTAL	INPUT AREA	CORR AREA	PCT OF TOTAL	AREA RATIO
82.0	3608.0	92.86	198.1	277.3	7.13	7.68
81.7	3594.8	92.85	197.5	276.5	7.14	7.69
81.8	3601.4	92.85	197.8	276.9	7.14	7.68

COMPUTER AREA RESULTS (THE LAST SET IS THE AVERAGE)

0.0	0.0	0.00	0.0	0.0	0.00	0.00
0.0	0.0	0.00	0.0	0.0	0.00	0.00
0.0	0.0	0.00	0.0	0.0	0.00	0.00

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H2S/SO2 SYSTEM

CALIBRATION SAMPLE NUMBER 12

SAMPLE PREPARATION CONDITIONS

ROOM TEMPERATURE..... 293.3 DEG K

BATH TEMPERATURE..... 292.7 DEG K

ATMOSPHERIC PRESSURE..... 703.1 MM HG

VOLUME OF NITROGEN..... 4619.3 CC

VOLUME OF HYDROGEN SULFIDE 215.1 CC

SAMPLE COMPOSITION (MOLE PERCENT)

NITROGEN..... 95.49

HYDROGEN SULFIDE... 4.50

100X MOLAR RATIO... 4.71

DISK INTEGRATOR AREA RESULTS (THE LAST SET IS THE AVERAGE)

NITROGEN			HYDROGEN SULFIDE			100X
INPUT AREA	CORR AREA	PCT OF TOTAL	INPUT AREA	CORR AREA	PCT OF TOTAL	AREA RATIO
80.3	3533.1	91.25	241.8	338.5	8.74	9.58
80.8	3555.1	91.23	244.0	341.6	8.76	9.60
80.5	3544.1	91.24	242.9	340.0	8.75	9.59

COMPUTER AREA RESULTS (THE LAST SET IS THE AVERAGE)

0.0	0.0	0.00	0.0	0.0	0.00	0.00
0.0	0.0	0.00	0.0	0.0	0.00	0.00
0.0	0.0	0.00	0.0	0.0	0.00	0.00

TABLE A-9

LEAST SQUARE FIT OF GC CALIBRATION DATA FOR H₂SH₂S/SO₂ SYSTEMX = AREA RATIO OF H₂S/N₂ (PERCENT)Y = MOLAR RATIO OF H₂S/SO₂ (PERCENT)

THE COEFFICIENTS OF THE FIRST ORDER POLYNOMIAL ARE

A₀ = -0.02980A₁ = 0.49192

REGENERATED DATA

X MEASURED	Y OBSERVED	Y CALCULATED	PCT ERROR
2.370	1.130	1.136	0.536
3.900	1.910	1.888	1.115
4.660	2.270	2.262	0.327
6.620	3.200	3.226	0.835
7.680	3.730	3.748	0.487
9.590	4.710	4.687	0.472

VARIANCE = 0.000417

STANDARD DEVIATION = 0.020424

MAXIMUM PCT ERROR = 1.115000

TABLE A-10

LEAST SQUARE FIT OF GC CALIBRATION DATA FOR SO₂
H₂S/SO₂ SYSTEM

X = AREA RATIO OF SO₂/N₂ (PERCENT)
Y = MOLAR RATIO OF SO₂/N₂ (PERCENT)

THE COEFFICIENTS OF THE FIRST ORDER POLYNOMIAL ARE

A₀ = 0.01775
A₁ = 0.43876

REGENERATED DATA

X MEASURED	Y OBSERVED	Y CALCULATED	PCT ERROR
1.300	0.580	0.588	1.404
2.660	1.180	1.184	0.411
3.700	1.640	1.641	0.071
4.130	1.850	1.829	1.089
4.710	2.110	2.084	1.216
5.570	2.430	2.461	1.302

VARIANCE = 0.000431
STANDARD DEVIATION = 0.020781
MAXIMUM PCT ERROR = 1.404182

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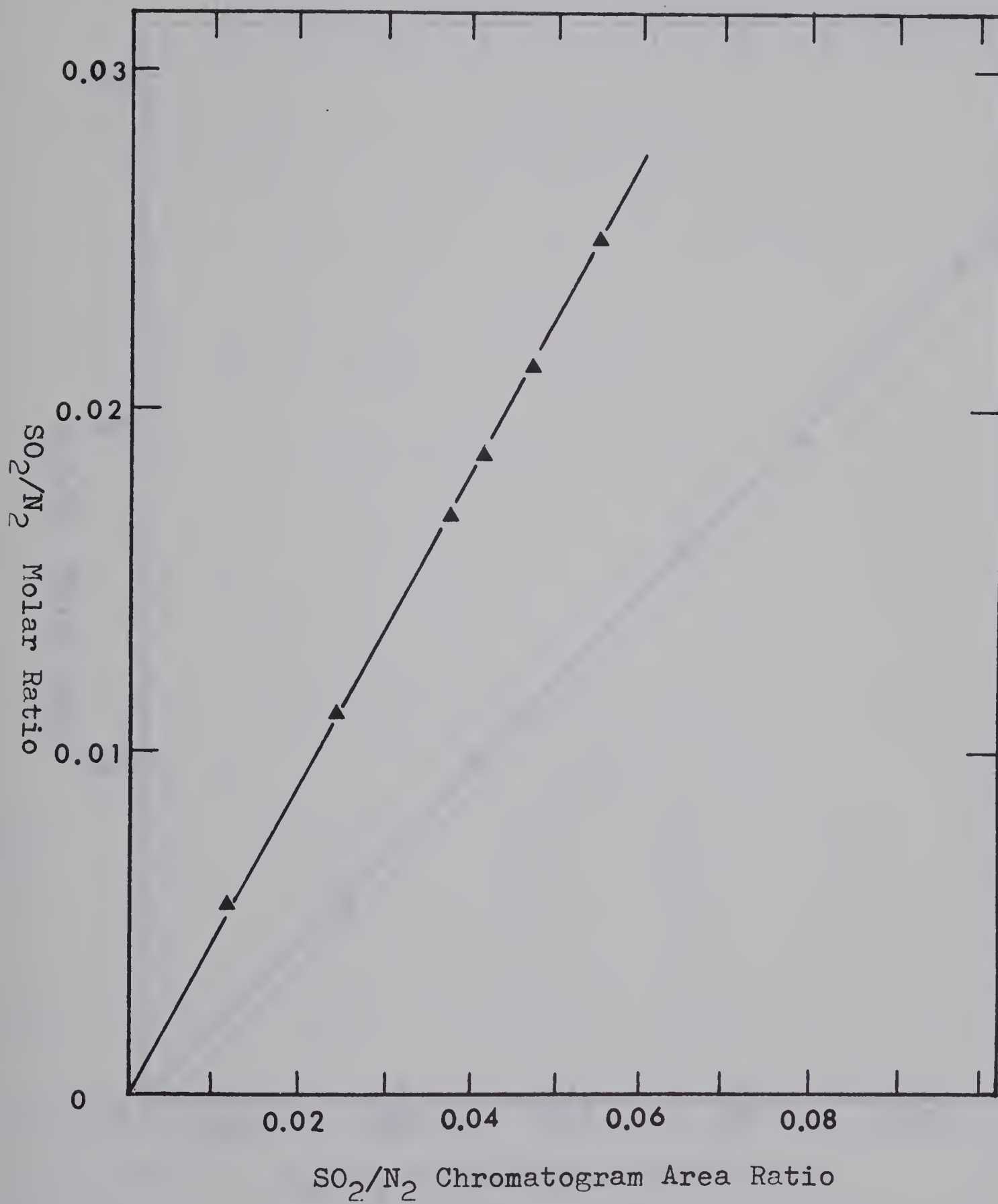


Figure A-3 Calibration of SO_2 Chromatogram for $\text{H}_2\text{S}/\text{SO}_2$ system

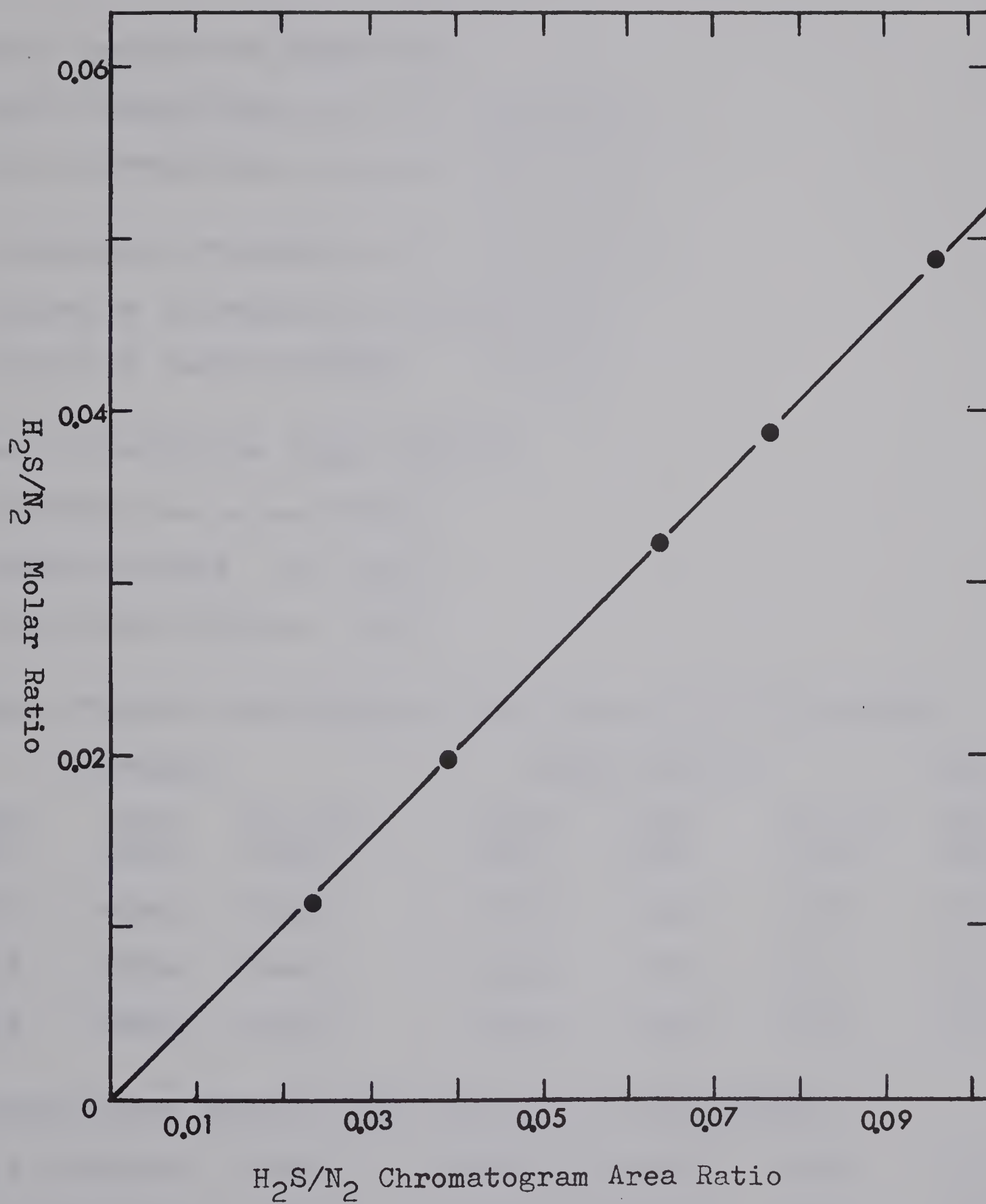


Figure A-4 Calibration of H_2S Chromatogram for H_2S/SO_2 system

COS/SO2 SYSTEM

CALIBRATION SAMPLE NUMBER 13

SAMPLE PREPARATION CONDITIONS

ROOM TEMPERATURE..... 294.4 DEG K

BATH TEMPERATURE..... 294.4 DEG K

ATMOSPHERIC PRESSURE..... 706.8 MM HG

VOLUME OF NITROGEN..... 3851.2 CC

VOLUME OF CARBON DIOXIDE 80.9 CC

SAMPLE COMPOSITION (MOLE PERCENT)

NITROGEN..... 97.93

CARBON DIOXIDE ... 2.06

100X MOLAR RATIO... 2.10

DISK INTEGRATOR AREA RESULTS (THE LAST SET IS THE AVERAGE)

NITROGEN			CARBON DIOXIDE			100X
INPUT AREA	CORR AREA	PCT OF TOTAL	INPUT AREA	CORR AREA	PCT OF TOTAL	AREA RATIO
98.0	3816.1	96.06	111.8	156.5	3.93	4.10
97.2	3784.9	96.05	111.0	155.4	3.94	4.10
97.6	3800.5	96.05	111.4	155.9	3.94	4.10

COMPUTER AREA RESULTS (THE LAST SET IS THE AVERAGE)

68171.8	2654609.9	95.96	79765.6	111671.9	4.03	4.20
67870.5	2642877.4	95.96	79446.7	111225.4	4.03	4.20
68021.1	2648743.4	95.96	79606.1	111448.7	4.03	4.20

COS/SO2 SYSTEM

CALIBRATION SAMPLE NUMBER 14

SAMPLE PREPARATION CONDITIONS

ROOM TEMPERATURE..... 294.4 DEG K

BATH TEMPERATURE..... 294.4 DEG K

ATMOSPHERIC PRESSURE..... 706.8 MM HG

VOLUME OF NITROGEN..... 3851.2 CC

VOLUME OF CARBON DIOXIDE 65.0 CC

SAMPLE COMPOSITION (MOLE PERCENT)

NITROGEN..... 98.33

CARBON DIOXIDE ... 1.66

100X MOLAR RATIO... 1.69

DISK INTEGRATOR AREA RESULTS (THE LAST SET IS THE AVERAGE)

NITROGEN			CARBON DIOXIDE			100X
INPUT AREA	CORR AREA	PCT OF TOTAL	INPUT AREA	CORR AREA	PCT OF TOTAL	AREA RATIO
98.8	3847.2	96.72	93.1	130.3	3.27	3.38
97.4	3792.7	96.69	92.6	129.6	3.30	3.41
98.1	3820.0	96.70	92.8	129.9	3.29	3.40

COMPUTER AREA RESULTS (THE LAST SET IS THE AVERAGE)

68859.0	2681369.4	96.63	66748.0	93447.3	3.36	3.48
68454.7	2665625.4	96.66	65609.0	91852.7	3.33	3.44
68656.8	2673497.4	96.65	66178.5	92650.0	3.34	3.46

COS/SO2 SYSTEM

CALIBRATION SAMPLE NUMBER 15

SAMPLE PREPARATION CONDITIONS

ROOM TEMPERATURE..... 295.0 DEG K

BATH TEMPERATURE..... 295.0 DEG K

ATMOSPHERIC PRESSURE..... 706.9 MM HG

VOLUME OF NITROGEN..... 3851.2 CC

VOLUME OF CARBON DIOXIDE 42.5 CC

SAMPLE COMPOSITION (MOLE PERCENT)

NITROGEN..... 98.90

CARBON DIOXIDE ... 1.09

100X MOLAR RATIO... 1.10

DISK INTEGRATOR AREA RESULTS (THE LAST SET IS THE AVERAGE)

NITROGEN			CARBON DIOXIDE			100X
INPUT AREA	CORR AREA	PCT OF TOTAL	INPUT AREA	CORR AREA	PCT OF TOTAL	AREA RATIO
94.6	3683.7	97.64	63.4	88.7	2.35	2.40
96.2	3746.0	97.61	65.3	91.4	2.38	2.44
95.4	3714.8	97.63	64.3	90.1	2.36	2.42

COMPUTER AREA RESULTS (THE LAST SET IS THE AVERAGE)

66657.4	2595638.9	97.55	46387.8	64942.9	2.44	2.50
67098.1	2612799.9	97.59	45948.7	64328.2	2.40	2.46
66877.7	2604219.4	97.57	46168.2	64635.6	2.42	2.48

COS/SO2 SYSTEM

CALIBRATION SAMPLE NUMBER 16

SAMPLE PREPARATION CONDITIONS

ROOM TEMPERATURE..... 294.4 DEG K

BATH TEMPERATURE..... 294.4 DEG K

ATMOSPHERIC PRESSURE..... 706.8 MM HG

VOLUME OF NITROGEN..... 3851.2 CC

VOLUME OF CARBON DIOXIDE 24.1 CC

SAMPLE COMPOSITION (MOLE PERCENT)

NITROGEN..... 99.37

CARBON DIOXIDE ... 0.62

100X MOLAR RATIO... 0.62

DISK INTEGRATOR AREA RESULTS (THE LAST SET IS THE AVERAGE)

NITROGEN			CARBON DIOXIDE			100X
INPUT AREA	CORR AREA	PCT OF TOTAL	INPUT AREA	CORR AREA	PCT OF TOTAL	AREA RATIO
99.6	3878.4	98.45	43.5	60.9	1.54	1.57
99.8	3886.2	98.41	44.6	62.4	1.58	1.60
99.6	3882.3	98.43	44.0	61.6	1.56	1.58

COMPUTER AREA RESULTS (THE LAST SET IS THE AVERAGE)

9378.6	2701602.4	98.41	31053.5	43474.9	1.58	1.60
9456.1	2704620.4	98.41	31111.1	43555.5	1.58	1.61
9417.3	2703111.4	98.41	31082.3	43515.2	1.58	1.60

COS/SO2 SYSTEM

CALIBRATION SAMPLE NUMBER 17

SAMPLE PREPARATION CONDITIONS

ROOM TEMPERATURE..... 295.0 DEG K

BATH TEMPERATURE..... 295.0 DEG K

ATMOSPHERIC PRESSURE..... 706.8 MM HG

VOLUME OF NITROGEN..... 3851.2 CC

VOLUME OF CARBON DIOXIDE 11.9 CC

SAMPLE COMPOSITION (MOLE PERCENT)

NITROGEN..... 99.69

CARBON DIOXIDE ... 0.30

100X MOLAR RATIO... 0.30

DISK INTEGRATOR AREA RESULTS (THE LAST SET IS THE AVERAGE)

NITROGEN			CARBON DIOXIDE			100X
INPUT AREA	CORR AREA	PCT OF TOTAL	INPUT AREA	CORR AREA	PCT OF TOTAL	AREA RATIO
99.5	3874.5	98.94	29.5	41.3	1.05	1.06
98.0	3816.1	98.94	29.0	40.6	1.05	1.06
98.7	3845.3	98.94	29.2	40.9	1.05	1.06

COMPUTER AREA RESULTS (THE LAST SET IS THE AVERAGE)

70026.7	2726839.4	98.96	20454.3	28636.0	1.03	1.05
69952.0	2723930.9	98.92	21095.1	29533.1	1.07	1.08
69989.3	2725384.9	98.94	20774.6	29084.6	1.05	1.06

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COS/SO2 SYSTEM

CALIBRATION SAMPLE NUMBER 18

SAMPLE PREPARATION CONDITIONS

ROOM TEMPERATURE..... 295.0 DEG K

BATH TEMPERATURE..... 295.0 DEG K

ATMOSPHERIC PRESSURE..... 701.2 MM HG

VOLUME OF NITROGEN..... 3851.2 CC

VOLUME OF CARBONYL SULFIDE 280.5 CC

SAMPLE COMPOSITION (MOLE PERCENT)

NITROGEN..... 93.21

CARBONYL SULFIDE... 6.78

100X MOLAR RATIO... 7.28

DISK INTEGRATOR AREA RESULTS (THE LAST SET IS THE AVERAGE)

NITROGEN			CARBONYL SULFIDE			100X
INPUT AREA	CORR AREA	PCT OF TOTAL	INPUT AREA	CORR AREA	PCT OF TOTAL	AREA RATIO
91.2	3551.3	89.29	193.6	425.9	10.70	11.99
91.0	3543.5	89.29	193.1	424.8	10.70	11.98
91.1	3547.4	89.29	193.3	425.3	10.70	11.99

COMPUTER AREA RESULTS (THE LAST SET IS THE AVERAGE)

66021.1	2570861.4	89.35	139161.1	306154.5	10.64	11.90
65603.7	2554608.9	89.38	137854.3	303279.5	10.61	11.87
65812.4	2562734.9	89.37	138507.7	304717.0	10.62	11.89

COS/SO2 SYSTEM

CALIBRATION SAMPLE NUMBER 19

SAMPLE PREPARATION CONDITIONS

ROOM TEMPERATURE..... 295.0 DEG K

BATH TEMPERATURE..... 295.0 DEG K

ATMOSPHERIC PRESSURE..... 701.2 MM HG

VOLUME OF NITROGEN..... 3851.2 CC

VOLUME OF CARBONYL SULFIDE 259.0 CC

SAMPLE COMPOSITION (MOLE PERCENT)

NITROGEN..... 93.69

CARBONYL SULFIDE... 6.30

100X MOLAR RATIO... 6.72

DISK INTEGRATOR AREA RESULTS (THE LAST SET IS THE AVERAGE)

NITROGEN			CARBONYL SULFIDE			100X
INPUT AREA	CORR AREA	PCT OF TOTAL	INPUT AREA	CORR AREA	PCT OF TOTAL	AREA RATIO
91.9	3578.5	89.95	181.6	399.5	10.04	11.16
91.4	3559.1	89.98	180.1	396.2	10.01	11.13
91.6	3568.8	89.96	180.8	397.8	10.03	11.14

COMPUTER AREA RESULTS (THE LAST SET IS THE AVERAGE)

66405.6	2585833.9	90.02	130217.6	286478.8	9.97	11.07
66188.4	2577375.9	90.01	129921.5	285827.4	9.98	11.08
66296.9	2581604.9	90.02	130069.5	286153.1	9.97	11.08

COS/SO2 SYSTEM

CALIBRATION SAMPLE NUMBER 20

SAMPLE PREPARATION CONDITIONS

ROOM TEMPERATURE..... 295.0 DEG K

BATH TEMPERATURE..... 295.0 DEG K

ATMOSPHERIC PRESSURE..... 701.1 MM HG

VOLUME OF NITROGEN..... 3851.2 CC

VOLUME OF CARBONYL SULFIDE 237.5 CC

SAMPLE COMPOSITION (MOLE PERCENT)

NITROGEN..... 94.19

CARBONYL SULFIDE... 5.80

100X MOLAR RATIO... 6.16

DISK INTEGRATOR AREA RESULTS (THE LAST SET IS THE AVERAGE)

NITROGEN			CARBONYL SULFIDE			100X
INPUT AREA	CORR AREA	PCT OF TOTAL	INPUT AREA	CORR AREA	PCT OF TOTAL	AREA RATIO
90.9	3539.6	90.91	160.7	353.5	9.08	9.98
90.7	3531.8	90.91	160.4	352.8	9.08	9.99
90.8	3535.7	90.91	160.5	353.2	9.08	9.98

COMPUTER AREA RESULTS (THE LAST SET IS THE AVERAGE)

65943.1	2567823.9	90.67	120037.1	264081.7	9.32	10.28
65781.2	2561519.4	90.92	116168.3	255570.3	9.07	9.97
65862.1	2564671.4	90.80	118102.7	259826.0	9.19	10.13

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COS/SO2 SYSTEM

CALIBRATION SAMPLE NUMBER 21

SAMPLE PREPARATION CONDITIONS

ROOM TEMPERATURE..... 294.4 DEG K

BATH TEMPERATURE..... 294.4 DEG K

ATMOSPHERIC PRESSURE..... 701.3 MM HG

VOLUME OF NITROGEN..... 3851.2 CC

VOLUME OF CARBONYL SULFIDE 118.1 CC

SAMPLE COMPOSITION (MOLE PERCENT)

NITROGEN..... 97.02

CARBONYL SULFIDE... 2.97

100X MOLAR RATIO... 3.06

DISK INTEGRATOR AREA RESULTS (THE LAST SET IS THE AVERAGE)

NITROGEN			CARBONYL SULFIDE			100X
INPUT AREA	CORR AREA	PCT OF TOTAL	INPUT AREA	CORR AREA	PCT OF TOTAL	AREA RATIO
94.0	3660.3	95.15	84.8	186.5	4.84	5.09
95.2	3707.0	95.18	85.2	187.4	4.81	5.05
94.6	3683.7	95.16	84.9	187.0	4.83	5.07

COMPUTER AREA RESULTS (THE LAST SET IS THE AVERAGE)

65934.5	2567489.4	95.15	59478.0	130851.6	4.84	5.09
67410.5	2624964.9	95.22	59767.3	131488.1	4.77	5.00
66672.5	2596226.9	95.19	59622.6	131169.8	4.80	5.05

COS/SO2 SYSTEM

CALIBRATION SAMPLE NUMBER 22

SAMPLE PREPARATION CONDITIONS

ROOM TEMPERATURE..... 295.0 DEG K

BATH TEMPERATURE..... 295.0 DEG K

ATMOSPHERIC PRESSURE..... 701.2 MM HG

VOLUME OF NITROGEN..... 3851.2 CC

VOLUME OF CARBONYL SULFIDE 67.8 CC

SAMPLE COMPOSITION (MOLE PERCENT)

NITROGEN..... 98.26

CARBONYL SULFIDE... 1.73

100X MOLAR RATIO... 1.76

DISK INTEGRATOR AREA RESULTS (THE LAST SET IS THE AVERAGE)

NITROGEN			CARBONYL SULFIDE			100X
INPUT AREA	CORR AREA	PCT OF TOTAL	INPUT AREA	CORR AREA	PCT OF TOTAL	AREA RATIO
95.3	3710.9	97.10	50.3	110.6	2.89	2.98
94.9	3695.4	97.10	50.1	110.2	2.89	2.98
95.1	3703.1	97.10	50.2	110.4	2.89	2.98

COMPUTER AREA RESULTS (THE LAST SET IS THE AVERAGE)

67310.2	2621058.9	97.13	35192.3	77423.0	2.86	2.95
67234.7	2618118.9	97.12	35284.0	77624.8	2.87	2.96
67272.4	2619588.9	97.12	35238.1	77523.9	2.87	2.95

COS/SO2 SYSTEM

CALIBRATION SAMPLE NUMBER 23

SAMPLE PREPARATION CONDITIONS

ROOM TEMPERATURE..... 294.4 DEG K

BATH TEMPERATURE..... 294.4 DEG K

ATMOSPHERIC PRESSURE..... 706.8 MM HG

VOLUME OF NITROGEN..... 3851.2 CC

VOLUME OF SULFUR DIOXIDE 151.1 CC

SAMPLE COMPOSITION (MOLE PERCENT)

NITROGEN..... 96.13

SULFUR DIOXIDE ... 3.86

100X MOLAR RATIO... 4.01

DISK INTEGRATOR AREA RESULTS (THE LAST SET IS THE AVERAGE)

NITROGEN			SULFUR DIOXIDE			100X
INPUT AREA	CORR AREA	PCT OF TOTAL	INPUT AREA	CORR AREA	PCT OF TOTAL	AREA RATIO
95.0	3699.3	92.51	383.5	299.1	7.48	8.08
96.9	3773.2	92.50	391.9	305.6	7.49	8.10
95.9	3736.2	92.51	387.7	302.4	7.48	8.09

COMPUTER AREA RESULTS (THE LAST SET IS THE AVERAGE)

65913.2	2566659.4	92.58	263524.4	205549.7	7.41	8.00
66500.5	2589529.4	92.58	265740.6	207278.3	7.41	8.00
66206.8	2578094.4	92.58	264632.4	206414.0	7.41	8.00

COS/SO2 SYSTEM

CALIBRATION SAMPLE NUMBER 24

SAMPLE PREPARATION CONDITIONS

ROOM TEMPERATURE..... 294.4 DEG K

BATH TEMPERATURE..... 294.4 DEG K

ATMOSPHERIC PRESSURE..... 706.8 MM HG

VOLUME OF NITROGEN..... 3851.2 CC

VOLUME OF SULFUR DIOXIDE 123.6 CC

SAMPLE COMPOSITION (MOLE PERCENT)

NITROGEN..... 96.81

SULFUR DIOXIDE ... 3.18

100X MOLAR RATIO... 3.28

DISK INTEGRATOR AREA RESULTS (THE LAST SET IS THE AVERAGE)

NITROGEN			SULFUR DIOXIDE			100X
INPUT AREA	CORR AREA	PCT OF TOTAL	INPUT AREA	CORR AREA	PCT OF TOTAL	AREA RATIO
95.1	3703.1	93.82	312.5	243.7	6.17	6.58
97.0	3777.1	93.64	328.5	256.2	6.35	6.78
96.0	3740.1	93.73	320.5	249.9	6.26	6.68

COMPUTER AREA RESULTS (THE LAST SET IS THE AVERAGE)

65979.1	2569225.9	93.79	218039.8	170071.6	6.20	6.61
66567.1	2592122.9	93.78	220196.7	171753.9	6.21	6.62
66273.1	2580674.4	93.78	219118.2	170912.8	6.21	6.62

COS/SO2 SYSTEM

CALIBRATION SAMPLE NUMBER 25

SAMPLE PREPARATION CONDITIONS

ROOM TEMPERATURE..... 293.8 DEG K

BATH TEMPERATURE..... 294.1 DEG K

ATMOSPHERIC PRESSURE..... 706.8 MM HG

VOLUME OF NITROGEN..... 3851.2 CC

VOLUME OF SULFUR DIOXIDE 94.8 CC

SAMPLE COMPOSITION (MOLE PERCENT)

NITROGEN..... 97.54

SULFUR DIOXIDE ... 2.45

100X MOLAR RATIO... 2.51

DISK INTEGRATOR AREA RESULTS (THE LAST SET IS THE AVERAGE)

NITROGEN			SULFUR DIOXIDE			100X
INPUT AREA	CORR AREA	PCT OF TOTAL	INPUT AREA	CORR AREA	PCT OF TOTAL	AREA RATIO
95.1	3703.1	95.27	235.3	183.5	4.72	4.95
95.3	3710.9	95.23	238.2	185.7	4.76	5.00
95.1	3707.0	95.25	236.7	184.6	4.74	4.98

COMPUTER AREA RESULTS (THE LAST SET IS THE AVERAGE)

67036.7	2610408.9	95.23	167431.1	130596.6	4.76	5.00
66792.0	2600880.4	95.28	164991.4	128693.7	4.71	4.94
66914.3	2605644.4	95.26	166211.2	129645.1	4.73	4.97

COS/SO2 SYSTEM

CALIBRATION SAMPLE NUMBER 26

SAMPLE PREPARATION CONDITIONS

ROOM TEMPERATURE..... 293.8 DEG K

BATH TEMPERATURE..... 294.4 DEG K

ATMOSPHERIC PRESSURE..... 706.8 MM HG

VOLUME OF NITROGEN..... 3851.2 CC

VOLUME OF SULFUR DIOXIDE 62.4 CC

SAMPLE COMPOSITION (MOLE PERCENT)

NITROGEN..... 98.37

SULFUR DIOXIDE ... 1.62

100X MOLAR RATIO... 1.65

DISK INTEGRATOR AREA RESULTS (THE LAST SET IS THE AVERAGE)

NITROGEN			SULFUR DIOXIDE			100X
INPUT AREA	CORR AREA	PCT OF TOTAL	INPUT AREA	CORR AREA	PCT OF TOTAL	AREA RATIO
93.2	3629.2	96.74	156.3	121.9	3.25	3.36
94.2	3668.1	96.74	158.2	123.3	3.25	3.36
93.7	3648.6	96.74	157.2	122.6	3.25	3.36

COMPUTER AREA RESULTS (THE LAST SET IS THE AVERAGE)

66256.6	2580031.9	96.76	110717.9	86360.2	3.23	3.34
66473.9	2588493.4	96.74	111782.6	87190.7	3.25	3.36
66365.2	2584262.4	96.75	111250.2	86775.4	3.24	3.35

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COS/SO2 SYSTEM

CALIBRATION SAMPLE NUMBER 27

SAMPLE PREPARATION CONDITIONS

ROOM TEMPERATURE..... 293.8 DEG K

BATH TEMPERATURE..... 294.4 DEG K

ATMOSPHERIC PRESSURE..... 706.8 MM HG

VOLUME OF NITROGEN..... 3851.2 CC

VOLUME OF SULFUR DIOXIDE 48.4 CC

SAMPLE COMPOSITION (MOLE PERCENT)

NITROGEN..... 98.73

SULFUR DIOXIDE ... 1.26

100X MOLAR RATIO... 1.28

DISK INTEGRATOR AREA RESULTS (THE LAST SET IS THE AVERAGE)

NITROGEN			SULFUR DIOXIDE			100X
INPUT AREA	CORR AREA	PCT OF TOTAL	INPUT AREA	CORR AREA	PCT OF TOTAL	AREA RATIO
95.1	3703.1	97.51	121.1	94.4	2.48	2.55
95.2	3707.0	97.52	120.6	94.1	2.47	2.53
95.1	3705.1	97.51	120.8	94.2	2.48	2.54

COMPUTER AREA RESULTS (THE LAST SET IS THE AVERAGE)

67448.8	2626456.4	97.43	88630.0	69131.6	2.56	2.63
67068.0	2611627.9	97.42	88609.8	69115.8	2.57	2.64
67258.4	2619041.9	97.42	88619.9	69123.7	2.57	2.63

TABLE A-11

LEAST SQUARE FIT OF CO₂ GC CALIBRATION DATA (DISK
INTEGRATER AREA)

THE COEFFICIENTS OF THE FIRST ORDER POLYNOMIAL ARE

A0 = -0.32264
A1 = 0.59102

REGENERATED DATA

X MEASURED	Y OBSERVED	Y CALCULATED	PCT ERROR
4.100	2.100	2.100	0.025
3.400	1.690	1.686	0.187
2.420	1.100	1.107	0.693
1.580	0.620	0.611	1.424
1.060	0.300	0.303	1.278

VARIANCE = 0.000040
STANDARD DEVIATION = 0.006348
MAXIMUM PCT ERROR = 1.424512

TABLE A-12

LEAST SQUARE FIT OF CO₂ GC CALIBRATION DATA (COMPUTER
INTEGRATED AREA)

THE COEFFICIENTS OF THE FIRST ORDER POLYNOMIAL ARE

A0 = -0.30699

A1 = 0.57382

REGENERATED DATA

X MEASURED	Y OBSERVED	Y CALCULATED	PCT ERROR
4.200	2.100	2.103	0.146
3.460	1.690	1.678	0.683
2.480	1.100	1.116	1.463
1.600	0.620	0.611	1.431
1.060	0.300	0.301	0.419

VARIANCE = 0.000120

STANDARD DEVIATION = 0.010981

MAXIMUM PCT ERROR = 1.463088

TABLE A-13

LEAST SQUARE FIT OF COS GC CALIBRATION DATA (DISK
INTEGRATER AREA)

THE COEFFICIENTS OF THE FIRST ORDER POLYNOMIAL ARE

A0 = -0.04980

A1 = 0.61295

REGENERATED DATA

X MEASURED	Y OBSERVED	Y CALCULATED	PCT ERROR
11.990	7.280	7.299	0.267
11.140	6.720	6.778	0.869
9.980	6.160	6.067	1.502
5.070	3.060	3.057	0.070
2.980	1.760	1.776	0.953

VARIANCE = 0.003162

STANDARD DEVIATION = 0.056237

MAXIMUM PCT ERROR

TABLE A-14

LEAST SQUARE FIT OF COS GC CALIBRATION DATA (COMPUTER
INTEGRATED AREA)

THE COEFFICIENTS OF THE FIRST ORDER POLYNOMIAL ARE

$$A_0 = -0.04747$$

$$A_1 = 0.61356$$

REGENERATED DATA

X MEASURED	Y OBSERVED	Y CALCULATED	PCT ERROR
11.890	7.280	7.247	0.442
11.080	6.720	6.750	0.458
10.130	6.160	6.167	0.128
5.050	3.060	3.051	0.293
2.950	1.760	1.762	0.143

VARIANCE = 0.000534

STANDARD DEVIATION = 0.023109

MAXIMUM PCT ERROR = 0.458132

TABLE A-15

LEAST SQUARE FIT OF SO₂ GC CALIBRATION DATA (DISK
INTEGRATER AREA)

THE COEFFICIENTS OF THE FIRST ORDER POLYNOMIAL ARE

A0 = 0.02306
A1 = 0.49180

REGENERATED DATA

X MEASURED	Y OBSERVED	Y CALCULATED	PCT ERROR
8.090	4.010	4.001	0.206
6.680	3.280	3.308	0.862
4.980	2.510	2.472	1.504
3.360	1.650	1.675	1.546
2.540	1.280	1.272	0.606

VARIANCE = 0.000751
STANDARD DEVIATION = 0.027415
MAXIMUM PCT ERROR = 1.546238

TABLE A-16

LEAST SQUARE FIT OF SO₂ GC CALIBRATION DATA (COMPUTER
INTEGRATED AREA)

THE COEFFICIENTS OF THE FIRST ORDER POLYNOMIAL ARE

A0 = -0.03956

A1 = 0.50558

REGENERATED DATA

X MEASURED	Y OBSERVED	Y CALCULATED	PCT ERROR
8.000	4.010	4.005	0.121
6.620	3.280	3.307	0.835
4.970	2.510	2.473	1.466
3.350	1.650	1.654	0.251
2.630	1.280	1.290	0.791

VARIANCE = 0.000562
STANDARD DEVIATION = 0.023714
MAXIMUM PCT ERROR = 1.466303

MAINLINE LEAST

```

C *****
C *
C *          MAINLINE LEAST
C *
C * THIS PROGRAM WAS WRITTEN FOR FITTING A MAXIMUM OF
C * 50 DATA POINTS TO POWER SERIES TYPE POLYNOMIALS OF
C * ANY ORDER UP TO A MAXIMUM OF FOURTH DEGREE.
C *   INPUT DATA
C *       NCASE  - NUMBER OF SETS OF DATA
C *       NCOPY  - NUMBER OF COPIES OF OUTPUT DESIRED
C *       N      - NUMBER OF DATA POINTS
C *       M      - DEGREE OF POLYNOMIAL
C *       NTL    - NUMBER OF CARDS FOR TITLE
C *       NPAGE  - PAGE NUMBER OF OUTPUT
C *       NPLT   - DATA REGENERATION FLAG
C *               ...0-REGENERATE GIVEN DATA ONLY
C *               ...1-REGENERATE GIVEN DATA PLUS 20
C *               INTERMEDIATE POINTS
C *       DES(K) - ALPHANUMERIC DESCRIPTION OF THE TITLE
C *       XNAME  - ALPHANUMERIC DESCRIPTION OF X
C *       YNAME  - ALPHANUMERIC DESCRIPTION OF Y
C *       X(I)   - INDEPENDENT VARIABLE
C *       Y(I)   - DEPENDENT VARIABLE
C *
C *****
C   DIMENSION X(50),Y(50),A(50,5),P(20,20),V(20),Z(20),
1  DES(10,15),SNAM(5),XNAME(100),YNAME(100)
C   DATA SNAM/'A0 =','A1 =','A2 =','A3 =','A4 ='/
C   READ(5,1) NCASE,NCOPY
C   DO 9 NC=1,NCASE
C   READ(5,1) N,M,NTL,NPAGE,NPLT
1  FORMAT(5I5)
C   DO 11 NT=1,NTL
11 READ(5,12) (DES(NT,K),K=1,15)
12 FORMAT(15A4)
C   READ (5,20) (XNAME(I),I=1,15)
20 FORMAT (15A4)
C   READ (5,21) (YNAME(J),J=1,15)
21 FORMAT (15A4)
13 FORMAT(10X,15A4/)
C   MM=M+1
C   DO 2 I=1,N
2  READ(5,3) X(I),Y(I)
3  FORMAT(2F10.5)
C   DO 4 I=1,N

```


MAINLINE LEAST(CONTINUED)

```

      DO 4 J=1,MM
4  A(I,J)=X(I)**(J-1)
      DO 5 I=1,MM
      DO 5 J=1,MM
      P(I,J)=0.
      DO 5 K=1,N
5  P(I,J)=P(I,J)+A(K,I)*A(K,J)
      DO 6 I=1,MM
      V(I)=0.
      DO 6 J=1,N
6  V(I)=V(I)+Y(J)*A(J,I)
      CALL GAUSS(P,V,MM,Z)
      DO 16 ICOP=1,NCOPY
      WRITE(6,10) NPAGE
10  FORMAT('1',///,66X,'A-',I2,/)
      DO 17 I=1,NTL
17  WRITE(6,13)(DES(I,K),K=1,15)
      WRITE (6,30) (XNAME(I),I=1,15)
30  FORMAT (///,12X,15A4)
      WRITE (6,31) (YNAME(J),J=1,15)
31  FORMAT (12X,15A4)
      WRITE(6,8)
8  FORMAT( ///,10X,'THE COEFFICIENTS OF THE POLYNOMIAL '
1, 'ARE$'/)
      DO 15 I=1,MM
15  WRITE(6,7) SNAM(I),Z(I)
7  FORMAT(15X,A4,F11.5/)
16  CALL REGEN(X,Y,Z,MM,N)
      IF(NPLT) 9,9,14
14  CALL POLYT (X,Z,N,MM)
9  CONTINUE
      CALL EXIT
      END

```

OT CONTROL STMT

D 27 APR 71 04.22.43

SUBROUTINE POLYT

```

C *****
C *
C *          SUBROUTINE POLYT
C *
C * POLYT SUPPLIES REGENERATED DATA AT POINTS INTER-
C * MEDIATE TO THE GIVEN DATA.
C *
C *****
SUBROUTINE POLYT(X,Z,N,MM)
DIMENSION X(50),Z(20)
WRITE(6,1)
1 FORMAT(///,32X,'PLOT TEST DATA'//25X'X CALCULATED',4X
1,'Y CALCULATED'/)
XMAX=0.
XMIN=99999.
DO 2 I=1,N
IF(XMAX-X(I)) 3,3,4
3 XMAX=X(I)
4 IF(X(I)-XMIN) 5,5,2
5 XMIN=X(I)
2 CONTINUE
DELX=(XMAX-XMIN)/20.
XY=XMIN
DO 6 I=1,20
CAL=0.
DO 15 J=1,MM
15 CAL=CAL+Z(J)*XY**(J-1)
WRITE(6,7) XY,CAL
7 FORMAT(24X,2(F10.3,5X))
6 XY=XY+DELX
RETURN
END

```


SUBROUTINE REGEN

```

C *****
C *
C *          SUBROUTINE REGEN
C *
C * THIS SUBROUTINE REGENERATES THE GIVEN DATA AND
C * CALCULATES THE VARIANCE AND STANDARD DEVIATION OF
C * THE FIT.
C *
C *****
SUBROUTINE REGEN(X,Y,Z,MM,N)
DIMENSION X(50),Y(50),Z(20)
WRITE(6,1)
1 FORMAT(///,29X,'REGENERATED DATA'//10X,'X MEASURED',5X
1,'Y OBSERVED',5X,'Y CALCULATED',3X,'PCT ERROR',/)
VAR=0.
HI=0.
DO 2 I=1,N
CAL=0.
DO 3 J=1,MM
3 CAL=CAL+Z(J)*X(I)**(J-1)
CAT=ABS(Y(I)-CAL)
PCE=CAT/Y(I)*100.
VAR=VAR+CAT**2
IF(HI-PCE)4,4,2
4 HI=PCE
2 WRITE(6,5) X(I),Y(I),CAL,PCE
5 FORMAT( 9X,4(F10.3,5X)/)
VAR=VAR/(N-1)
DEV=VAR**0.5
WRITE(6,6) VAR,DEV,HI
6 FORMAT(//,10X'VARIANCE' =',F10.6//10X,
1'STANDARD DEVIATION =',F10.6//10X,
2'MAXIMUM PCT ERROR  =',F10.6)
RETURN
END

```


SUBROUTINE GAUSS

```

C      ****
C      *
C      *      SUBROUTINE GAUSS
C      *
C      * THE FUNCTION OF THIS SUBROUTINE IS TO SOLVE THE
C      * SET OF EQUATIONS  $A \cdot X = B$  USING GAUSSIAN ELIMINATION
C      * AND BACK SUBSTITUTION ROTATING ABOUT THE ELEMENT
C      * OF MAXIMUM MODULUS.
C      *
C      ****
SUBROUTINE GAUSS (A,R,N,X)
DIMENSION A(20,20),R(20),X(20)
M=N-1
DO 11 J=1,M
  S=0.
  DO 12 I=J,N
    U= ABS(A(I,J))
    IF(U-S) 12,12,112
112  S=U
    L=I
  12 CONTINUE
  IF(L-J) 119,19,119
119  DO 14 I=J,N
    S=A(L,I)
    A(L,I)=A(J,I)
  14  A(J,I)=S
    S=R(L)
    R(L)=R(J)
    R(J)=S
  19  IF( ABS(A(J,J))-1.E-30) 115,115,15
115  WRITE(6,3)
    GO TO 500
  15  MM=J+1
    DO 11 I=MM,N
      IF( ABS(A(I,J))-1.E-30) 11,111,111
111  S=A(J,J)/A(I,J)
    A(I,J)=0.0
    DO 16 K=MM,N
      16  A(I,K)=A(J,K)-S*A(I,K)
      R(I)=R(J)-S*R(I)
  11 CONTINUE
  DO 17 K=1,N
    I=N+1-K
    S=0.0
    IF(I-N) 117,17,117

```


SUBROUTINE GAUSS.....(CONTINUED)

```
117 MM=I+1
    DO 18 J=MM,N
18  S=S+A(I,J)*X(J)
17  X(I)=(R(I)-S)/A(I,I)
500 RETURN
    3  FORMAT (1H , 'MATRIX SINGULAR')
    END
```

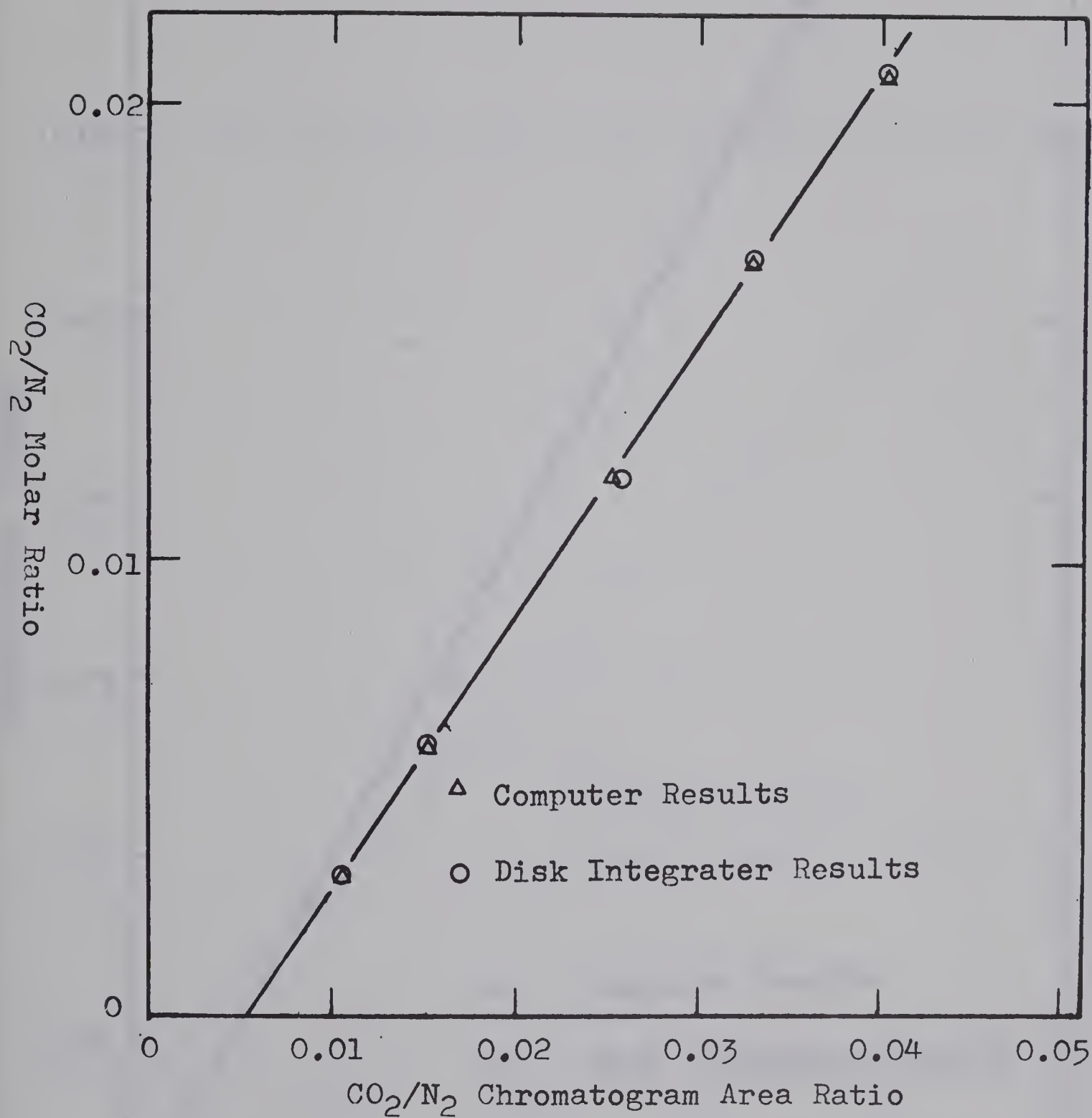



Figure A-5 Calibration of CO_2 Chromatogram for COS/SO_2 System

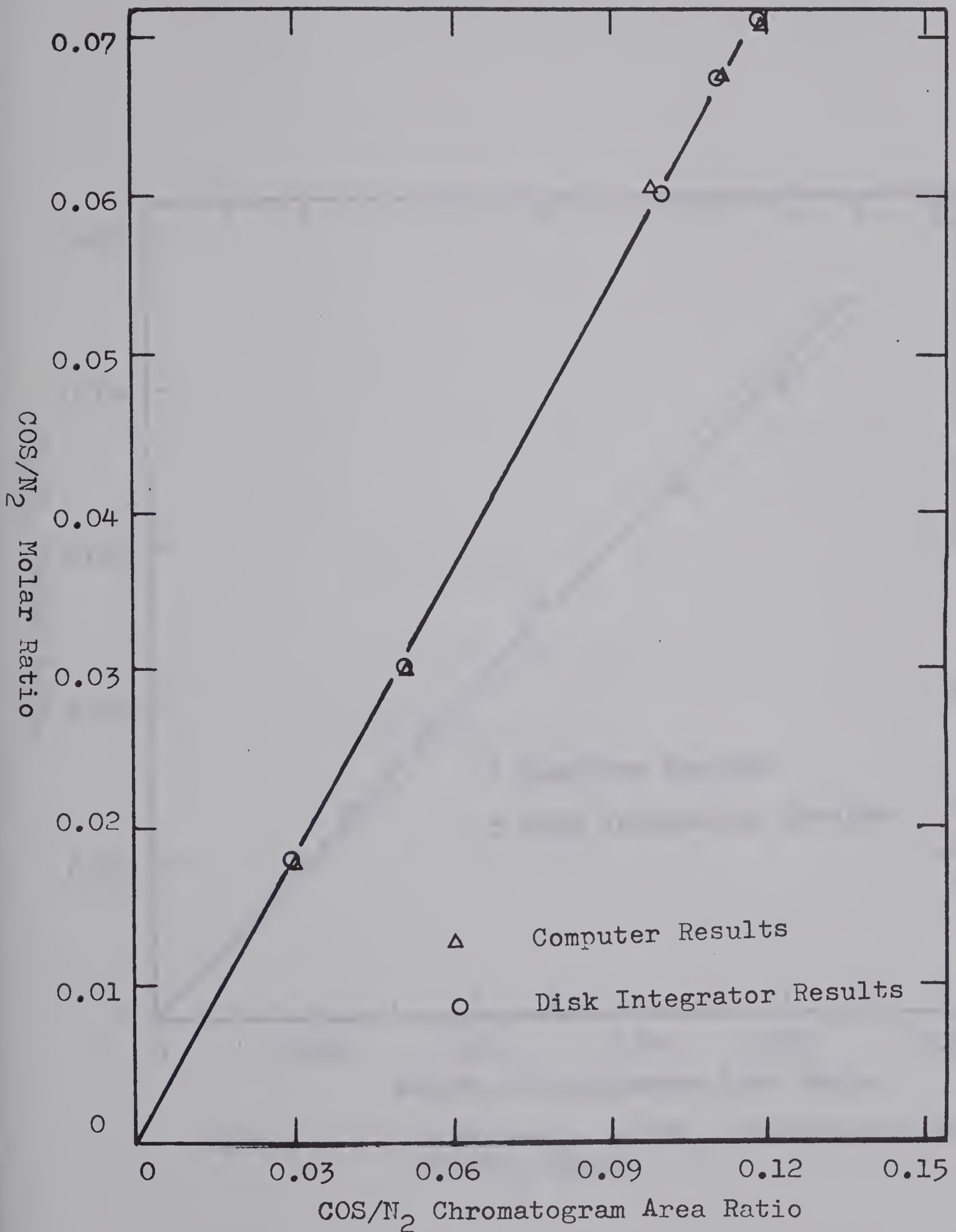


Figure A-6 Calibration of COS Chromatogram for COS/SO₂ System

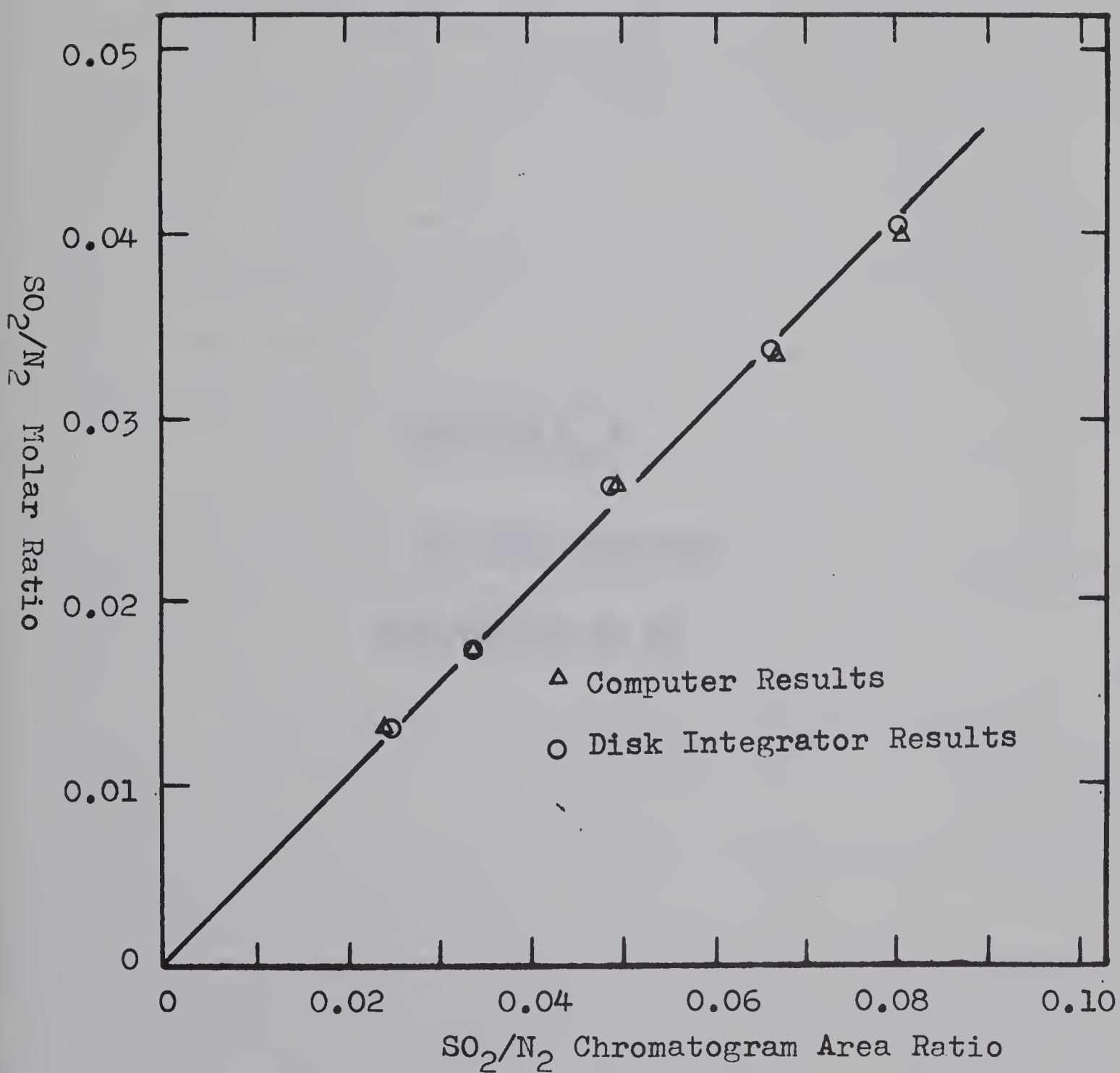


Figure A-7 Calibration of SO_2 Chromatogram for COS/SO_2 System

APPENDIX B

ON-LINE COMPUTER

MONITORING OF GC

B-I On-line GC Data Acquisition and Reduction

A generalized set of programs for computer monitoring of the gas chromatograph was written by McCollough^{*}. Coxhead^{**} attempted to modify the program so that it would simultaneously monitor the analog output of four gas chromatographs. In these programs, six scan parameters are required, which the user must specify to adjust the rejection dead band width applied to the chromatograph analog signal. Much trial-and-error manipulation of the parameters was needed in order to obtain the correct parameters.

Owing to the difficulties in trying out the parameters, in the present work an attempt was made to build a simple computer program which would monitor one gas chromatograph for one particular analysis.

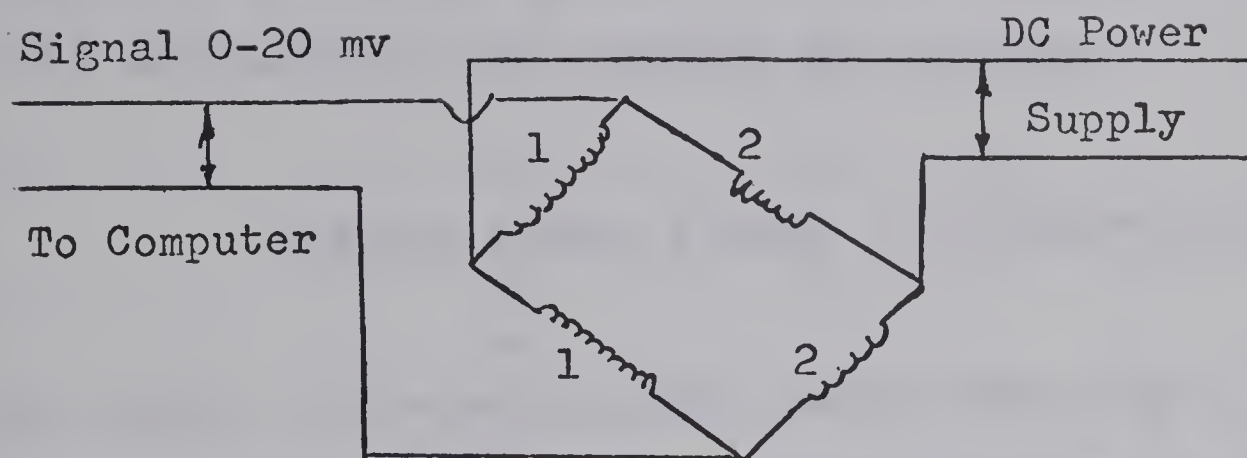
Only the approach used in developing the GC computer program and the interrelations of the functions performed by the computer program as well as peripheral devices will be described.

* McCollough, J., J. Gas Chromatography, 5(12), 635-40, 1967

** Coxhead, P., Master of Science thesis, University of Alberta, 1968

B-II Basic Logic of Computer Monitoring of GC Analog Signal

As shown in figure B-1, when a gas chromatograph senses a sample with its thermal conductivity cell detector, a potential difference is generated across the bridge circuit between the reference and detecting filaments. This potential difference can be transmitted to a gas chromatograph recorder and/or to a computer as well. The signal sent by the gas chromatograph to computer is analog, but for a digital computer such as the IBM-1800, digital data are stored. Therefore, the analog signal from the gas chromatograph has to be converted into a digital signal before it is received by the computer. Usually an analog-to-digital converter is used to perform this function. The ADC (analog-to-digital converter) is situated between the CPU (central processing unit) of the computer and peripheral device. Several types of ADC are available, each corresponding to different ranges of analog signal. For the present study, a 0-20 mv ADC was used. Voltages from the gas chromatograph must fall within this range before passing through the ADC. For the 16-bit word type IBM-1800



Key: 1. Detector Filement
2 Reference Resistances

Figure B-1 Gas Chromatograph Bridge Circuit

computer, the largest integer expressed by a "word" is 32767. Therefore a 20 mv analog signal will be stored in the computer as 32767 and a signal of V mv will be stored in the computer in the form

$$\text{Digital number stored} = (V)(32767)/(20)$$

The number of analog signals transmittable by a peripheral device to the computer per unit time is variable. In the present work, the speed is supervised and controlled by a built-in program called direct digital control (DDC) program. This program allows the fastest speed to be one signal per second. An example of the signals sent by the gas chromatograph to the computer and stored in the computer as numbers in 450 seconds is shown in figure B-2. Due to the large number of data stored in the computer during that period of time, the data were printed out in terms of 5 seconds, interval only. From the numbers shown, we can see that three peaks had been sensed by the gas chromatograph.

212	212	213	211	213	214	212	213	337	2054
412	215	214	213	212	213	355	539	1615	1423
1147	820	540	376	339	268	212	212	213	214
213	212	214	215	212	214	215	211	214	213
212	214	212	216	213	212	214	213	215	214
215	213	212	212	212	213	212	212	249	288
338	376	420	467	508	559	600	549	471	411
369	328	299	246	220	216	214	215	212	212
212	212	212	212	214	212	213	212	212	212

Figure B-2 Digital Print-Out of GC Signal by
Computer

B-III Development of On-line GC Computer Program

Before the GC monitoring program can be built, it is necessary to understand how the computer "sees" a gas chromatograph peak. Figure B-3 shows plots of typical ideal Gaussian peak and its first derivative. When the GC signal starts a peak, the first derivative of signal changes from zero to positive. At the point of maximum peak height, the first derivative changes from positive to zero. As soon as the peak goes down-slope, the first derivative becomes negative. Thus, to define a peak apex, we need to confirm the change from positive to negative of the first derivative. The first derivative returns to zero from negative as soon as the GC signal returns to the original baseline i.e. the peak ends.

By calculating the first derivative and confirming the completion of the cycle of the first derivative from zero to positive, from positive to zero, from zero to negative and from negative to zero, the computer is able to detect a peak.

Each data point received by the computer from the gas chromatograph is not processed immediately but rather, all data points corresponding to a particular GC analysis are received and stored in memory. Data processing can be commenced as soon as all data have

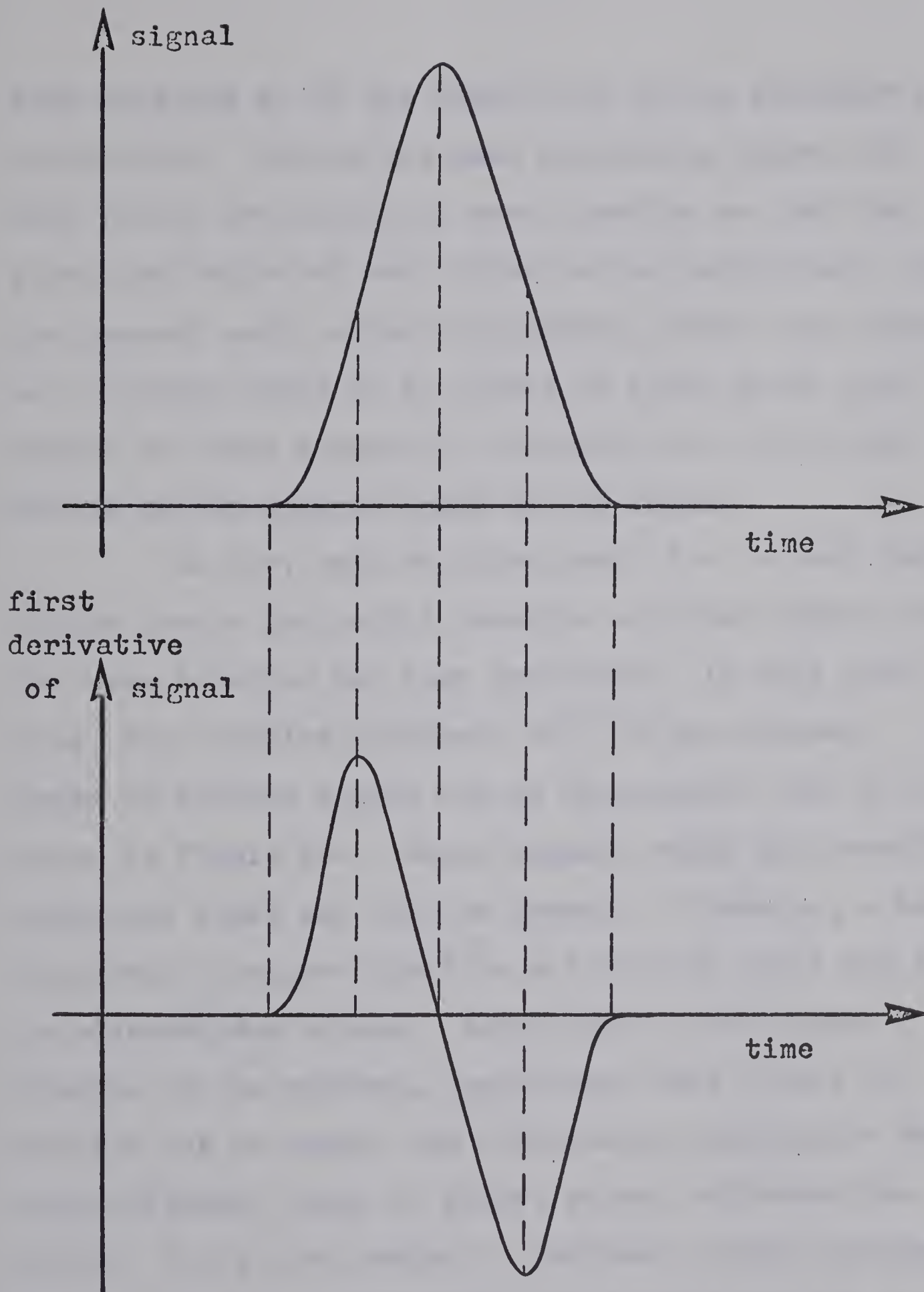


Figure B-3 Gas Chromatograph Peak and its First Derivative

been received or at any later time at the operator's convenience. During the data processing phase, all data points are fitted to some function so that the first derivative at each point can be calculated. In the present work, seven consecutive points were taken on a running basis to be fitted to third order polynomial by least squares to calculate the first derivative at the central point of the seven.

So far, only an ideal peak, i.e. a peak that starts from a horizontal baseline and then returns to the same baseline has been mentioned. In real practice, more complex phenomena will be encountered. Peaks of various shapes may be encountered such as those shown in figure B-4. Noise signals which may resemble component peaks may also be present. Moreover, a baseline drift from one level to a different level may also be mistaken for a peak. Before the GC monitoring program can be written, preliminary test should be carried out to enable the computer to distinguish between different forms of peaks, noise, and base-line drift. It is also useful to include a simple program for the computer instructing it to print out all the numerical data which it received from the GC before any GC signal detection program is built. An example of such a print-out is shown in figure B-2. From the print-out, the least elution time for the expected

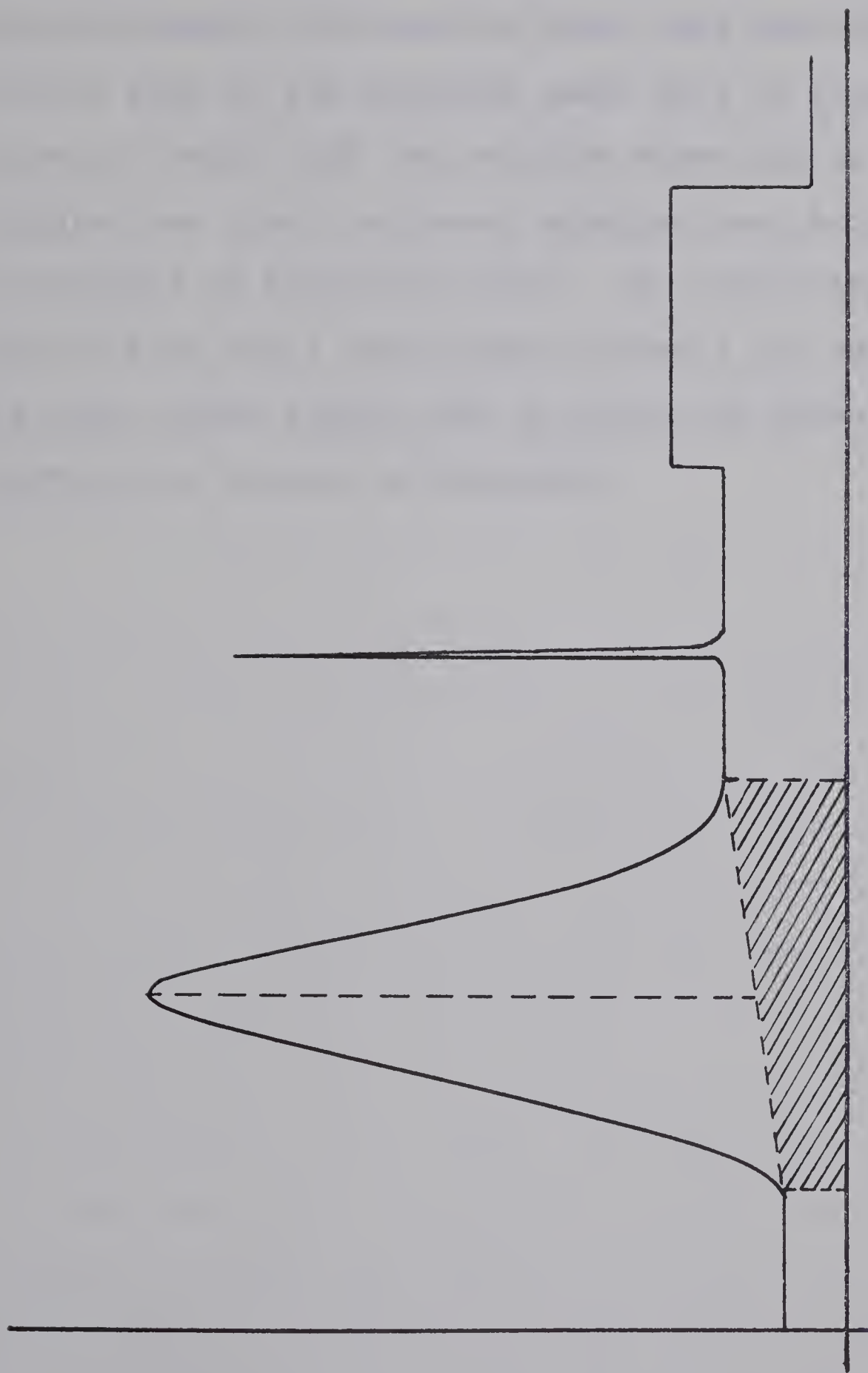


Figure B-4 Different Types of Gas Chromatograph Peaks

peaks as well as the lowest peak height can be determined. Signals (peaks) with elution times less than the least elution time of the expected peaks will be regarded as noise and peaks with long elution times but of peak heights less than the lowest expected peak height will be regarded as base-line drift. By specifying an elution time and a peak height criteria for each desirable peak, other signals due to noise and base-line drift can be ignored by computer.

B-IV Development of Program to Integrate GC Peak
Signals and Calculate Sample Compositions

Although the separation obtained with a particular GC column is sometimes calibrated in terms of relative peak heights verses known composition of the sample, relative peak area is used for calibration in most cases. Therefore, the computer needs to calculate the area under peaks which have been detected.

A number of ways are available in defining peak areas but only one method will be described in detail. In the present study, a fundamental base-line signal was obtained from a Leeds-Northrup model 8686 millivolt potentiometer, to enable the computer to receive a baseline signal without the presence of a peak signal. To calculate a peak area, the area below the base-line signal (shaded portion in figure B-4) should be deducted from the total area obtained by integrating a peak signal. As indicated in figure B-4, the true area of the peak is the difference between the total area and the trapezoidal area formed by the base-line signal from peak start to peak end. The total area was calculated using Simpson's Rule.

If a GC separation has been calibrated as a function of relative composition as,

$$\text{Relative composition} = f(\text{Relative peak area})$$

i.e.

$$\text{Relative composition} = \frac{\text{Mole fraction of component } i}{\text{Mole fraction of component } j}$$

where component j = a reference component

and if the function f, has been built into the computer program, the computer will then be able to calculate the composition from the integrated area.

Since a GC recorder can only give peak signals and peak areas, this program is greatly superior to the GC recorder. A listing of this GC program is shown in Appendix A.

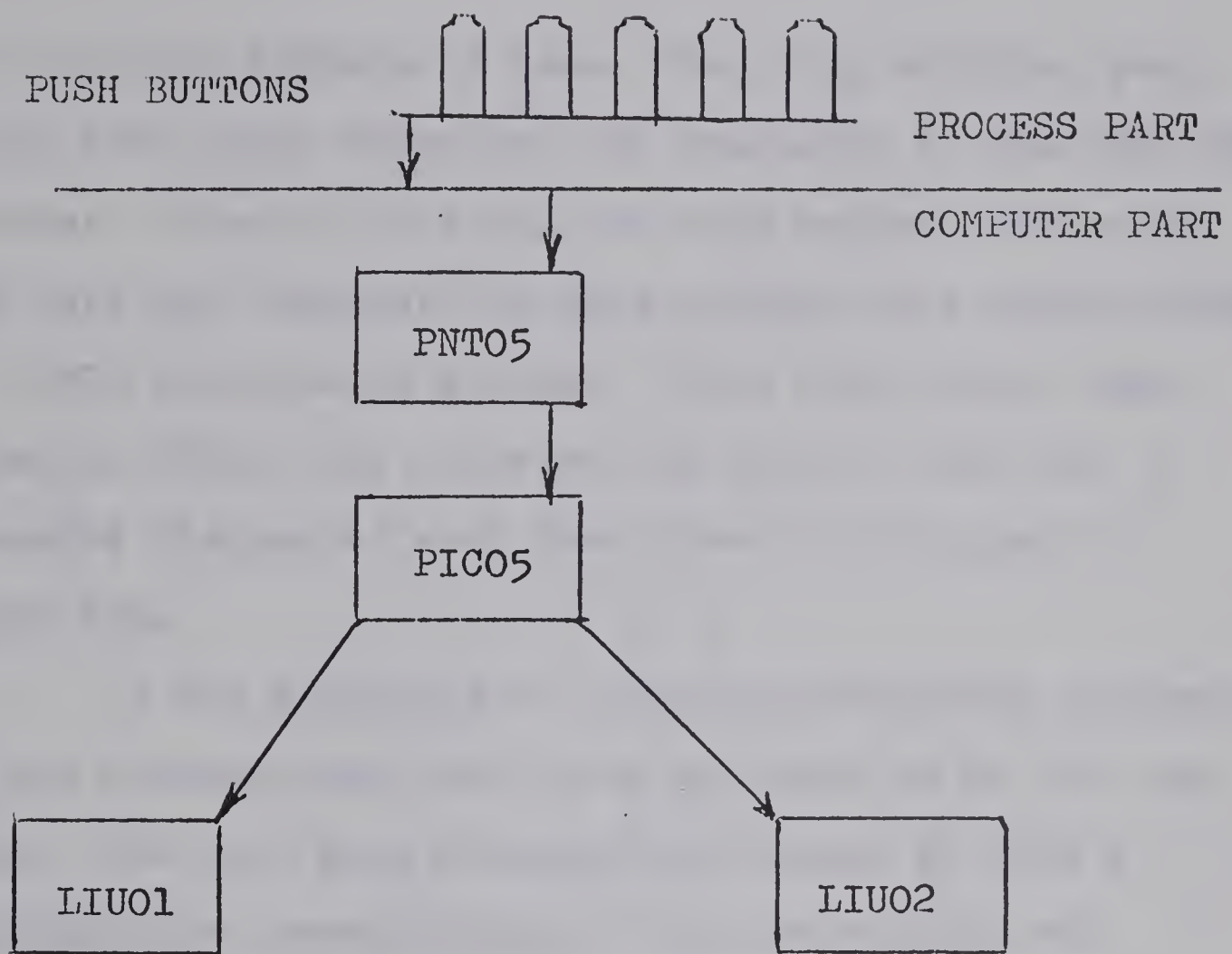
B-V On-line Operation of the GC and IBM-1800 System

Various combinations of on or off positions for four electric switches can be used to transmit signals representing coded instructions to the computer. In the present study, five electric push buttons were used to perform such one-way communication functions. When the online operation was to be started, one of five push buttons, called the interrupt button, was used to interrupt the computer so that the coded instructions on the remaining four switches could be acknowledged. The different combinations of on-off positions for the four switches represented different instructions. Each instruction could cause a program to be executed by the computer.

In the present work, when the interrupt button was pushed a program named PNT05 responded to the interrupt and queued a program named PIC05. PIC05 evaluated the position of the first of the remaining four push buttons. Since there were only two positions, namely on and off for that push button, one of the two programs stored in the computer related to this push button may be queued. These two programs were named LIU01 and LIU02. LIU01 monitored the GC operations and acquired and reduced the GC data. LIU02 stored the

processed or unprocessed data into a file or retrieved some data from a file. Each of the functions performed by LIU01 or LIU02 was carried out by a subprogram. Usually LIU01 or LIU02, when queued by PIC05, evaluated the configurations of the remaining three push buttons and then decided which subprogram to be called upon to execute different jobs. Figure B-5 indicates the flow of instructions from the online application to the computer.

The above topics are explained in more detail by considering a specific gas chromatograph analysis. Before proceeding further, it is necessary to discuss how gas chromatograph data are received and stored by DDC. DDC receives data from peripheral devices via loop records. Each loop record comprises a loop ID (which is essentially a name or identification of the data source), a number of words in a loop, and the speed of data transmission, etc . Two types of loop records are available in DDC for each data source, namely, data acquisition loop record and data accumulation loop record. The data acquisition loop record acquires data from peripheral devices and stores these in the data accumulation loop record. Data accumulation loop record then empties the data to ring buffer when it has been filled. The ring buffer is a location



Turn ECO on

Zero Accumulation
Loop Record

Turn on Acquisition
and Accumulation
Loop Records

Retrieve
and
Process
GC Data

Turn Loop
Records Off

Figure B-5 On-line GC Program Flow Diagram

for temporary storage of data. Two ring buffers, each of 120 data point capacity, are available in the IBM-1800 computer. When it is full, the ring buffer empties the data into the computer DDC data storage file named DAFLE. The DAFLE contains 64 sectors. Each data point, when stored in DAFLE file, carries the loop ID with it. A schematic diagram of such data flow is indicated in figure B-6.

At the beginning of a gas chromatograph analysis the gas chromatograph has to be switched on by the computer. The four push buttons are pressed to form a configuration corresponding to the instruction of switching on the GC by the computer. The interrupt button is pushed so that computer will receive the instruction. After the interrupt button is pushed, the program PNT05 is executed and a current signal is sent from the computer to the push button in the laboratory indicating that the interrupt has been acknowledged. At the same time, PNT05 queues a program named PIC05 to call upon another program to turn on the ECO (electric contact operation) which is equivalent to turning on the GC. The ECO turns on GC by energizing the microswitch on the GC programmer which sustains the power supply to the cam motor drive. It takes 10 seconds to energize and start the cam motor, therefore,

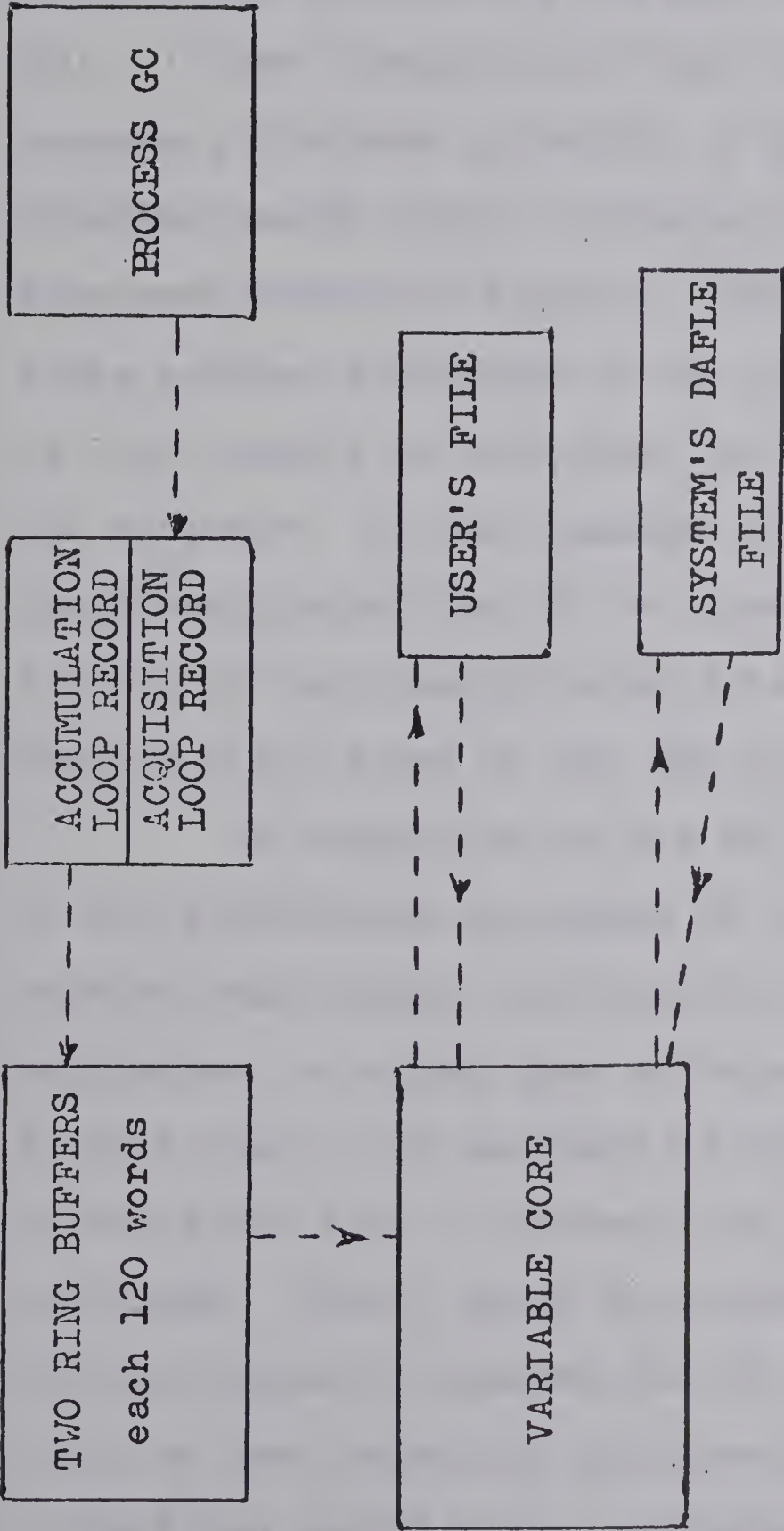


Figure B-6 DDC Data Flow Diagram

ECO is turned on for 15 seconds, and then turned off by the same program. Figure 12-A shows the cam system and figure 12-B depicts the electrical network involved in interfacing the cam drive motor with the ECO. If gas chromatograph data are to be sent to the computer, the same procedure of pressing buttons is repeated except that a different configuration of the four push button is applied. This configuration will cause another subprogram to be called upon to turn on loop records so that data can be transferred to the computer. If the transfer of data needs to be done immediately after the GC is turned on, the program for turning on loop records should be built into the subprogram which turns on the ECO and GC.

On completion of the GC analysis, a repetition of the push-button procedure is again carried out, with another push-button configuration such that another subprogram is called upon to turn off loop record. At this stage, the complete GC analysis data are stored in the DAFLE file. However, the data are still not processed. Hence, again by pushing buttons, a program will be queued to process the GC data according to the logic of peak detection and area integration and sample composition calculations mentioned earlier.

After the GC data are processed, another subprogram can be called upon to store the processed

data in the user's file. Raw data in DAFLE file can be cleared. The loop records pointers are reset to their original position. All of these functions are also performed by pushing buttons.

Figure B-5 shows the interrelations of the programs and functions performed. The various devices and instruments used to carry out GC analysis and the way they are interconnected are shown in figure B-7.

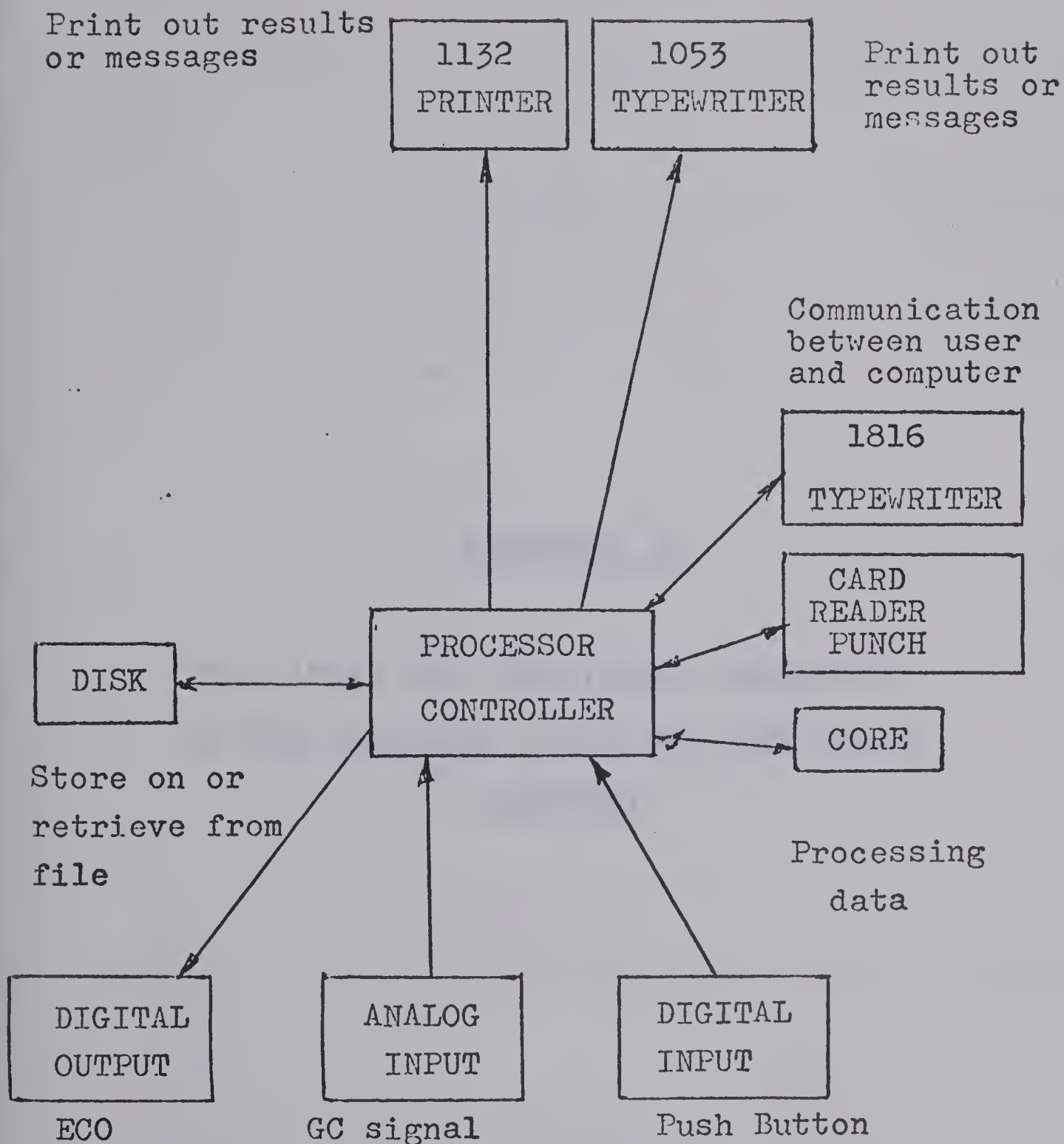


Figure B-7 IBM-1800 Computer and Peripheral
Devices for On-line GC Monitor

APPENDIX C

TO EXAMINE THE EQUILIBRIUM CONVERSION
OF THE REACTIONS INVOLVING SOME SULFUR
COMPOUND

MAINLINE FREM

```

C *****
C *
C *          MAINLINE PREM
C *
C * THIS PROGRAM CALCULATES EQUILIBRIUM COMPOSITIONS
C * FOR COMPLEX REACTION SYSTEMS USING THE FREE ENERGY
C * MINIMIZATION METHOD DEVELOPED BY WHITE AND
C * COWORKERS. IT WILL HANDLE UP TO TWENTY DIFFERENT
C * ELEMENTS. ANY NUMBER OF CASES CAN BE ATTEMPTED WITH
C * COWORKERS. IT WILL HANDLE UP TO TWENTY DEFFERENT
C * AS MANY TEMPERATURES AND PRESSURES DESIRED.
C *
C * INPUT DATA
C *      M      - NUMBER OF DIFFERENT ELEMENTS
C *      N      - NUMBER OF GASEOUS SPECIES
C *      P      - NUMBER OF CONDENSED SPECIES
C *      NPT    - NUMBER OF TEMP. AND PRESS. CONDITIONS
C *      SNAM   - THE NAMES OF THE SPECIES
C *      X      - THE AMOUNT OF THIS SPECIE PRESENT IN
C *               THE STARTING CHEMICAL SYSTEM (EITHER
C *               NUMBER OF MOLES OR MOLE FRACTION)
C *      A      - SPECIE ROW IN MASS BALANCE CONSTRAINT
C *      FRE    - COEFFICIENTS FOR FREE ENERGY EXPRESSION
C *      PRESS  - PRESSURE (ATMOSPHERES)
C *      T      - TEMPERATURE (DEGREES KELVIN)
C *
C *****
C      INTEGER P
C      DIMENSION SNAM(20,5),FRE(20,7),X(20),GA(20,20),GB(20),
1,F(20),A(20,20),Y(20),B(20),FRC(20),NG1(20),XX(20)
C      READ(5,1) M,N,P,NPT
1  FORMAT(5I5)
C      N2=N+P
C      DO 2 I=1,N2
C      READ(5,3) (SNAM(I,K),K=1,5),X(I)
C      WRITE(6,3)(SNAM(I,K),K=1,5),X(I)
3  FORMAT(1X,A3,4A4, F15.7)
C      READ(5,4) (A(I,J),J=1,M)
C      WRITE(6,4)(A(I,J),J=1,M)
4  FORMAT( 7(3X,F7.2))
C      READ(5,5) (FRE(I,K),K=1,7)
2  WRITE(6,6) (FRE(I,K),K=1,7)
5  FORMAT (5E15.7)
6  FORMAT (1X,4E15.7)
C      DO 101 II=1,14

```


MAINLINE FREM(CONTINUED)

```

101 XX(II)=X(II)
    WRITE(6,7)
7  FORMAT(1H1,40X,'FREE ENERGY MINIMIZATION'///30X,'MOLE'
1  'ULAR SPECY'10X'INITIAL MOLE NUMBERS',10X,'INITIAL MO
1,/)
    CALL DISTR(X,Y,B,N2,M,A)
    CALL MOFR(Y,FRC,N,P)
    DO 8 I=1,N2
8  WRITE(6,9) (SNAM(I,K),K=1,5),Y(I),FRC(I)
9  FORMAT(30X,A3,4A4,10X,E15.7,10X,E15.7,/)
    JBI=2
    DO 10 NC=1,NPT
    READ(5,11)PRESS,T
11  FORMAT(5F10.5)
    DO 12 I=1,N2
    NG1(I)=0
    FRT=FRE(I,1)*(1.-ALOG(T))-FRE(I,2)*T/2.-FRE(I,3)*T**2/
1.-FRE(I,4)*T**3/12.-FRE(I,5)*T**4/20.+FRE(I,6)/T-FRE(I
1,7)
    C(I)=FRT+ALOG(PRESS)
    IF(I-N)12,12,13
13  C(I)=FRT
12  CONTINUE
    DO 35 JB=1,JBI
    DO 14 ITER=1,300
    CALL FREN (Y,C,F,YBAR,N,P,NG1)
    MG=M+P+1
    CALL GSET (A,Y,GA,GB,B,F,P,M,MG,N)
    CALL GAUSS(GA,GB,MG,GX)
    IF(P)15,15,16
16  DO 17 I=1,P
    II=I+1
    IC=N+I
17  X(IC)=GX(II)
15  CONTINUE
    DO 18 I=1,N
    IF(NG1(I)) 19,19,18
19  X(I)=-Y(I)*((C(I)+ALOG(Y(I)/YBAR))-GX(1))
    DO 21 J=1,M
    IG=P+J+1
21  X(I)=X(I)+GX(IG)*A(I,J)*Y(I)
18  CONTINUE
    CALL NEZE (X,Y,N2,NG1)
    QUIT=1.
    DO 22 I=1,N2

```


MAINLINE FREM(CONTINUED)

```

      IF(NG1(I)) 23,23,22
23  TEST=(X(I)-Y(I))/X(I)
      IF(ABS(TEST)-0.1E-03) 22,22,24
24  QUIT=-1.
22  CONTINUE
      IF(QUIT) 25,25,26
25  DO 27 I=1,N2
27  Y(I)=X(I)
14  CONTINUE
26  DO 32 I=1,N2
      NG1(I)=0
      IF(X(I)) 33,33,34
34  Y(I)=X(I)
      GO TO 32
33  Y(I)=0.000001
32  CONTINUE
35  CONTINUE
      WRITE(6,28)T,PRESS
28  FORMAT(1H1,28X'TEMPERATURE (DEG K)=' ,F7.1,5X,'PRESSU',
1'RE (ATM)=' ,F6.2/)
      WRITE(6,29) ITER
29  FORMAT (1H0,30X,'NUMBER OF ITERATION =' ,I5///30X,'MOLE
U,8X,'EQUILIBRIUM MOLE NUMBERS',8X,'MOLE FRATION'//)
      CALL MOFR (X,FRC,N,P)
      DO 30 I=1,N2
30  WRITE(6,31) (SNAM(I,K),K=1,5),X(I),FRC(I)
31  FORMAT (30X,A3,4A4,10X,E15.7,10X,E15.7,/)
      CALL COND (X,XX)
      JBI=1
10  CONTINUE
      STOP
      END

```


SUBROUTINE GSET

```

C *****
C *
C *          SUBROUTINE GSET
C *
C * THIS SUBROUTINE SETS UP THE MATRIX EQUATION WHICH
C * CORRESPONDS TO EQUATION 2.13 IN THE REVIEW OF THE
C * METHOD. THIS MATRIX EQUATION IS SOLVED USING
C * SUBROUTINE GAUSS.
C *
C *****
SUBROUTINE GSET (A,Y,GA,GB,B,F,P,M,MG,N)
  INTEGER P
  DIMENSION R(20,20),A(20,20),Y(20),GA(20,20),GB(20),B(2
  DO 1 K=1,M
  DO 1 J=1,K
  R(J,K)=0.0
  DO 2 I=1,N
2  R(J,K)=R(J,K)+A(I,J)*A(I,K)*Y(I)
1  R(K,J)=R(J,K)
  DO 3 I=1,MG
  DO 3 J=1,MG
3  GA(I,J)=0.0
  DO 4 IG=1,M
  DO 5 I=1,N
5  GA(IG,1)=GA(IG,1)+A(I,IG)*Y(I)
  IF(P)6,6,7
7  DO 8 I=1,P
  JG=I+1
  JGG=IG+P+1
  IGG=I+M+1
  II=N+I
  GA(IG,JG)=A(II,IG)
8  GA(IGG,JGG)=GA(IG,JG)
6  CONTINUE
  DO 9 J=1,M
  JG=J+P+1
9  GA(IG,JG)=R(IG,J)
  JG=P+IG+1
  IGG=M+1
4  GA(IGG,JG)=GA(IG,1)
  DO 10 J=1,M
  GB(J)=B(J)
  DO 10 I=1,N
10 GB(J)=GB(J)+A(I,J)*F(I)
  JGB=M+1

```


SUBROUTINE GSET(CONTINUED)

```
      GB(JGB)=0.0
      DO 11 I=1,N
11    GB(JGB)=GB(JGB)+F(I)
      IF(P)12,12,13
13    DO 14 I=1,P
      JGB=M+I+1
      II=N+I
14    GB(JGB)=F(II)
12    CONTINUE
      RETURN
      END
```


SUBROUTINE GAUSS

```

C *****
C *
C *          SUBROUTINE GAUSS
C *
C * THE FUNCTION OF THIS SUBROUTINE IS TO SOLVE THE
C * SET OF EQUATIONS A*X=B USING GAUSSIAN ELIMINATION
C * AND BACK SUBSTITUTION ROTATING ABOUT THE ELEMENT
C * OF MAXIMUM MODULUS.
C *
C *****
SUBROUTINE GAUSS (A,R,N,X)
DIMENSION A(20,20),R(20),X(20)
M=N-1
DO 11 J=1,M
  S=0.
  DO 12 I=J,N
    U= ABS(A(I,J))
    IF(U-S) 12,12,112
112  S=U
    L=I
  12 CONTINUE
  IF(L-J) 119,19,119
119  DO 14 I=J,N
    S=A(L,I)
    A(L,I)=A(J,I)
  14  A(J,I)=S
    S=R(L)
    R(L)=R(J)
    R(J)=S
  19  IF( ABS(A(J,J))-1.E-30) 115,115,15
115  WRITE(6,3)
    3  FORMAT (1H ,'MATRIX SINGULAR')
    RETURN
  15  MM=J+1
    DO 11 I=MM,N
      IF( ABS(A(I,J))-1.E-30) 11,111,111
111  S=A(J,J)/A(I,J)
    A(I,J)=0.0
    DO 16 K=MM,N
      16  A(I,K)=A(J,K)-S*A(I,K)
      R(I)=R(J)-S*R(I)
  11 CONTINUE
  DO 17 K=1,N
    I=N+1-K
    S=0.0

```


SUBROUTINE GAUSS.....(CONTINUED)

```
      IF(I-N) 117,17,117
117  MM=I+1
      DO 18 J=MM,N
18   S=S+A(I,J)*X(J)
17   X(I)=(R(I)-S)/A(I,I)
      RETURN
      END
```


SUBROUTINE NEZE

```

*****
*
*               SUBROUTINE NEZE
*
* THIS SUBROUTINE TESTS FOR NEGATIVE OR ZERO AMOUNTS
* OF MOLECULAR SPECIES AND TAKES THE CORRECTIVE
* ACTION AS INDICATED IN THE METHOD REVIEW.
*
*****
SUBROUTINE NEZE (X,Y,N2,NG1)
DIMENSION X(20),Y(20),NG1(20)
TEST=1.0
DO 1 I=1,N2
  IF(NG1(I)) 2,2,1
2  IF(X(I)) 3,3,1
3  SLAM=-0.99*Y(I)/(X(I)-Y(I))
  IF(SLAM-TEST)4,4,1
4  TEST=SLAM
1  CONTINUE
DO 5 I=1,N2
  IF(NG1(I))7,7,5
7  X(I)=Y(I)+TEST*(X(I)-Y(I))
  IF(X(I)-0.10E-10) 6,6,5
6  X(I)=0.0
  NG1(I)=1
5  CONTINUE
RETURN
END

```


SUBROUTINE FREN

```

C *****
C *
C *          SUBROUTINE FREN
C *
C * THIS SUBROUTINE CALCULATES THE FREE ENERGY
C * CONTRIBUTION OF EACH SPECIE TO THE SYSTEM.
C *
C *****
SUBROUTINE FREN (Y,C,F,YBAR,N,P,NG1)
  INTEGER P
  DIMENSION Y(20),C(20),F(20),NG1(20)
  YBAR=0.0
  DO 1 I=1,N
1  YBAR=YBAR+Y(I)
  DO 2 I=1,N
    IF(NG1(I)) 3,3,4
3  F(I)=Y(I)*(C(I)+ALOG(Y(I)/YBAR))
    GO TO 2
4  F(I)=0.0
2  CONTINUE
    IF(P) 10,10,6
6  DO 7 I=1,P
    II=N+I
    IF(NG1(II)) 8,8,9
8  F(II)=Y(II)*C(II)
    GO TO 7
9  F(II)=0.0
7  CONTINUE
10 CONTINUE
    RETURN
  END

```


SUBROUTINE DISTR

```

C *****
C *
C *          SUBROUTINE DISTR
C *
C * THIS SUBROUTINE IS USED TO GENERATE A POSITIVE SET
C * OF MOLE NUMBERS FOR ALL SPECIES IN THE SYSTEM.
C *
C *****
SUBROUTINE DISTR(X,Y,B,N2,M,A)
DIMENSION X(20),Y(20),B(20),A(20,20)
DO 1 I=1,N2
  IF(X(I)) 2,2,1
2  X(I)=0.0000001
1  Y(I)=X(I)
  DO 3 J=1,M
    B(J)=0.0
  DO 3 I=1,N2
3  B(J)=B(J)+A(I,J)*Y(I)
  RETURN
END

```


SUBROUTINE MOFR

```

C *****
C *
C *          SUBROUTINE MOFR
C *
C * THIS PROGRAM CALCULATES THE MOLE FRACTION OF EACH
C * SPECIE IN THE MIXTURE
C *
C *****
SUBROUTINE MOFR (Y,FRC,N,P)
  INTEGER P
  DIMENSION Y(20),FRC(20)
  DEN=0.0
  DO 1 I=1,N
1  DEN=DEN+Y(I)
  DO 2 I=1,N
2  FRC(I)=Y(I)/DEN
  IF(P) 7,7,8
8  DEN=0.0
  DO 3 I=1,P
  II=N+I
3  DEN=DEN+Y(II)
  DO 4 I=1,P
  II=N+I
4  FRC(II)=Y(II)/DEN
7  CONTINUE
  RETURN
  END

```


SUBROUTINE COND

```

C *****
C *
C *          SUBROUTINE COND
C *
C * THIS PROGRAM CALCULATES THE PERCENTAGE OF
C * EQUILIBRIUM CONVERSION
C *
C *****
SUBROUTINE COND(X,XX)
DIMENSION X(20),XX(20)
CONV=(XX(1)-X(1))/XX(1)
WRITE(6,1) CONV
1 FORMAT(28X,'EQUILIBRIUM CONVERSION OF A (PCT)=' ,F6.3, /
RETURN
END

```


TABLE C- 1

EQUILIBRIUM PRODUCT DISTRIBUTION OF CLAUS REACTION USING
A TYPICAL FEED FROM WASTE HEAT BOILER OF SULFUR PLANT

MOLECULAR SPECIE	FEED MOLE FRACTION	EQUILIBRIUM MOLE FRACTION AT DIFFERENT TEMPERATURE (DEG. K)						
		300.0	350.0	400.0	450.0	500.0	550.0	600.0
H2S	0.0670	0.0056	0.0056	0.0056	0.0057	0.0059	0.0072	0.0102
SO2	0.0387	0.0000	0.0000	0.0000	0.0000	0.0001	0.0008	0.0023
COS	0.0095	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
CS2	0.0032	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
CO	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
CO2	0.0770	0.0919	0.0919	0.0919	0.0919	0.0918	0.0917	0.0915
H2O	0.0000	0.0630	0.0630	0.0630	0.0630	0.0627	0.0613	0.0582
H2	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
N2	0.8045	0.8246	0.8245	0.8244	0.8242	0.8237	0.8228	0.8213
SS	0.0000	0.0149	0.0147	0.0144	0.0136	0.0121	0.0098	0.0072
SE	0.0000	0.0000	0.0002	0.0006	0.0017	0.0037	0.0063	0.0089
S2	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0004
S1	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000

PCT. OF
-2S CONV.

91.320 91.810 91.800 91.760 91.400 89.470 85.140

TABLE C- 2

EQUILIBRIUM PRODUCT DISTRIBUTION OF CLAUS REACTION USING
A TYPICAL FEED FROM WASTE HEAT BOILER OF SULFUR PLANT

MOLECULAR SPECIE	FEED MOLE FRACTION	EQUILIBRIUM MOLE FRACTION AT DIFFERENT TEMPERATURE (DEG. K)							
		650.0	700.0	750.0	800.0	850.0	900.0	950.0	
H2S	0.0670	0.0143	0.0190	0.0234	0.0257	0.0252	0.0235	0.0218	
SO2	0.0387	0.0044	0.0068	0.0091	0.0104	0.0103	0.0096	0.0090	
COS	0.0095	0.0000	0.0001	0.0002	0.0004	0.0005	0.0006	0.0007	
CS2	0.0032	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	
CO	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0002	0.0005	
CO2	0.0770	0.0912	0.0907	0.0898	0.0886	0.0879	0.0876	0.0872	
H2O	0.0000	0.0539	0.0488	0.0439	0.0407	0.0408	0.0423	0.0438	
H2	0.0000	0.0000	0.0000	0.0000	0.0001	0.0001	0.0002	0.0004	
N2	0.8046	0.8190	0.8149	0.8079	0.7989	0.7942	0.7930	0.7925	
S2	0.0000	0.0047	0.0027	0.0011	0.0002	0.0000	0.0000	0.0000	
S6	0.0000	0.0106	0.0105	0.0078	0.0032	0.0005	0.0001	0.0000	
S2	0.0000	0.0019	0.0063	0.0168	0.0317	0.0403	0.0429	0.0441	
S1	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	
PCT. OF H2S CONV.		79.100	71.960	65.270	61.310	61.880	64.390	66.940	

TABLE C- 3

2COS = CO2 + CS2

TEMP. (DEG. K)	EQUIL. CONV. (PCT)	COS	CO2	CS2
300.0	59.82	0.8036	0.5982	0.5982
350.0	58.45	0.8310	0.5845	0.5845
400.0	57.39	0.8522	0.5739	0.5739
450.0	56.54	0.8692	0.5654	0.5654
500.0	55.84	0.8831	0.5584	0.5584
550.0	55.26	0.8948	0.5526	0.5526
600.0	54.76	0.9047	0.5476	0.5476
650.0	54.33	0.9133	0.5433	0.5433
700.0	53.96	0.9208	0.5396	0.5396
750.0	53.63	0.9275	0.5363	0.5363
800.0	53.33	0.9333	0.5333	0.5333
850.0	53.07	0.9386	0.5307	0.5307
900.0	52.83	0.9434	0.5283	0.5283
950.0	52.61	0.9478	0.5261	0.5261
1000.0	52.41	0.9517	0.5241	0.5241

TABLE C- 4



TEMP. (DEG. K)	EQUIL. CONV. (PCT)	SO2	CH4	H2S	CO	H2
300.0	0.00	1.00000	2.00000	0.00000	0.00000	0.00000
350.0	0.00	1.00000	2.00000	0.00000	0.00000	0.00000
400.0	6.18	0.93820	1.87640	0.06180	0.12360	0.18540
450.0	19.88	0.80120	1.60240	0.19880	0.39760	0.59640
500.0	46.85	0.53150	1.06300	0.46850	0.93690	1.40520
550.0	76.10	0.23900	0.47800	0.76100	1.52200	2.28300
600.0	91.63	0.09370	0.16740	0.91630	1.83250	2.74890
650.0	97.07	0.02930	0.05850	0.97070	1.94140	2.91220
700.0	98.67	0.01130	0.02250	0.98870	1.97740	2.96620
750.0	99.52	0.00480	0.00960	0.99520	1.99030	2.98550
800.0	99.77	0.00230	0.00460	0.99770	1.99540	2.99320
850.0	99.92	0.00120	0.00240	0.99880	1.99770	2.99640
900.0	99.93	0.00070	0.00140	0.99930	1.99860	2.99800
950.0	99.96	0.00040	0.00060	0.99960	1.99920	2.99880
1000.0	99.98	0.00020	0.00040	0.99980	1.99950	2.99930

TABLE C- 5

H2S = H2 + 1/X SX (X=ATOMIC NO. OF DIFF. S SPECIE)

TEMP. (DEG. K)	EQUILM. CONV. (PCT)	EQUILIBRIUM DISTRIBUTION					
		H2S	S8	S6	S2	S1	H2
300.0	0.00	1.0000	0.0000	0.0000	0.0000	0.0000	0.0000
350.0	0.00	1.0000	0.0000	0.0000	0.0000	0.0000	0.0000
400.0	0.00	1.0000	0.0000	0.0000	0.0000	0.0000	0.0000
450.0	0.00	1.0000	0.0000	0.0000	0.0000	0.0000	0.0000
500.0	0.00	1.0000	0.0000	0.0000	0.0000	0.0000	0.0000
550.0	0.03	0.9997	0.0000	0.0000	0.0000	0.0000	0.0003
600.0	0.06	0.9994	0.0000	0.0001	0.0000	0.0000	0.0006
650.0	0.12	0.9988	0.0000	0.0001	0.0003	0.0000	0.0012
700.0	0.23	0.9977	0.0000	0.0000	0.0010	0.0000	0.0023
750.0	0.43	0.9957	0.0000	0.0000	0.0021	0.0000	0.0043
800.0	0.78	0.9922	0.0000	0.0000	0.0039	0.0000	0.0078
850.0	1.32	0.9868	0.0000	0.0000	0.0066	0.0000	0.0132
900.0	2.10	0.9790	0.0000	0.0000	0.0105	0.0000	0.0210
950.0	2.90	0.9710	0.0000	0.0000	0.0145	0.0000	0.0290
1000.0	3.80	0.9620	0.0000	0.0000	0.0192	0.0000	0.0380

TABLE C- 6 CS2 + H2O = CO + H2S + 1/X SX (X=ATOMIC NO. OF DIFF. S SPECIE)

TEMP. (DEG. K)	EQUILM. CONV. (PCT)	EQUILIBRIUM DISTRIBUTION								
		CS2	H2O	CO	H2S	S8	S6	S2	S1	
300.0	66.28	0.3372	0.3372	0.6628	0.6628	0.0828	0.0001	0.0000	0.0000	
350.0	70.99	0.2901	0.2901	0.7099	0.7099	0.0882	0.0008	0.0000	0.0000	
400.0	74.20	0.2580	0.2580	0.7420	0.7420	0.0905	0.0030	0.0000	0.0000	
450.0	76.50	0.2350	0.2350	0.7650	0.7650	0.0893	0.0085	0.0000	0.0000	
500.0	78.23	0.2177	0.2177	0.7823	0.7823	0.0837	0.0188	0.0000	0.0000	
550.0	79.60	0.2040	0.2040	0.7960	0.7960	0.0738	0.0343	0.0002	0.0000	
600.0	80.73	0.1927	0.1927	0.8073	0.8073	0.0609	0.0530	0.0012	0.0000	
650.0	81.70	0.1830	0.1830	0.8170	0.8170	0.0471	0.0715	0.0058	0.0000	
700.0	82.57	0.1743	0.1743	0.8257	0.8257	0.0339	0.0854	0.0212	0.0000	
750.0	83.42	0.1658	0.1658	0.8342	0.8342	0.0218	0.0890	0.0632	0.0000	
800.0	84.37	0.1563	0.1563	0.8437	0.8437	0.0110	0.0742	0.1552	0.0000	
850.0	85.67	0.1433	0.1433	0.8567	0.8567	0.0032	0.0395	0.2972	0.0000	
900.0	87.47	0.1253	0.1253	0.8747	0.8747	0.0004	0.0102	0.4053	0.0000	
950.0	89.33	0.1067	0.1067	0.8933	0.8933	0.0000	0.0017	0.4413	0.0000	
1000.0	90.88	0.0912	0.0912	0.9088	0.9088	0.0000	0.0003	0.4535	0.0000	

TABLE C- 7 CS2 + CO2 = 2CO + 2/X SX (X=ATOMIC NO. OF DIFF. S SPECIE)

TEMP. (DEG. K)	EQUILV. CONV. (PCT)	EQUILIBRIUM DISTRIBUTION						
		CS2	CO2	S8	S6	S2	S1	CO
300.0	0.00	1.0000	1.0000	0.0000	0.0000	0.0000	0.0000	0.0000
350.0	0.00	1.0000	1.0000	0.0000	0.0000	0.0000	0.0000	0.0000
400.0	0.00	1.0000	1.0000	0.0000	0.0000	0.0000	0.0000	0.0000
450.0	0.00	1.0000	1.0000	0.0000	0.0000	0.0000	0.0000	0.0000
500.0	0.00	1.0000	1.0000	0.0000	0.0000	0.0000	0.0000	0.0000
550.0	0.00	1.0000	1.0000	0.0000	0.0000	0.0000	0.0000	0.0000
600.0	0.00	1.0000	1.0000	0.0000	0.0000	0.0000	0.0000	0.0000
650.0	0.00	1.0000	1.0000	0.0000	0.0000	0.0000	0.0000	0.0000
700.0	0.00	1.0000	1.0000	0.0000	0.0000	0.0000	0.0000	0.0000
750.0	0.00	1.0000	1.0000	0.0000	0.0000	0.0000	0.0000	0.0000
800.0	0.00	1.0000	1.0000	0.0000	0.0000	0.0000	0.0000	0.0000
850.0	0.00	1.0000	1.0000	0.0000	0.0000	0.0000	0.0000	0.0000
900.0	0.00	1.0000	1.0000	0.0000	0.0000	0.0000	0.0000	0.0000
950.0	0.00	1.0000	1.0000	0.0000	0.0000	0.0000	0.0000	0.0000
1000.0	0.00	1.0000	1.0000	0.0000	0.0000	0.0000	0.0000	0.0000

TABLE C- 8 SO2 + 2H2 = 1/X SX + 2H2O (X=ATOMIC NO. OF DIFF. S SPECIE)

TEMP. (DEG. K)	EQUILY. CONV. (PCT)	EQUILIBRIUM DISTRIBUTION						
		SO2	H2	S8	S6	S2	S1	H2O
300.0	100.00	0.0000	0.0000	0.1249	0.0002	0.0000	0.0000	2.0000
350.0	100.00	0.0000	0.0000	0.1243	0.0010	0.0000	0.0000	2.0000
400.0	100.00	0.0000	0.0000	0.1222	0.0038	0.0000	0.0000	2.0000
450.0	100.00	0.0000	0.0000	0.1172	0.0105	0.0000	0.0000	2.0000
500.0	100.00	0.0000	0.0000	0.1079	0.0228	0.0000	0.0000	2.0000
550.0	100.00	0.0000	0.0000	0.0940	0.0412	0.0002	0.0000	2.0000
600.0	99.98	0.0002	0.0005	0.0771	0.0634	0.0013	0.0000	1.9995
650.0	99.94	0.0006	0.0012	0.0594	0.0854	0.0062	0.0000	1.9988
700.0	99.87	0.0012	0.0026	0.0427	0.1020	0.0226	0.0000	1.9974
750.0	99.74	0.0026	0.0053	0.0276	0.1068	0.0668	0.0000	1.9947
800.0	99.52	0.0048	0.0095	0.0143	0.0908	0.1679	0.0000	1.9905
850.0	99.21	0.0079	0.0158	0.0044	0.0505	0.3271	0.0000	1.9842
900.0	98.82	0.0118	0.0236	0.0005	0.0134	0.4518	0.0000	1.9764
950.0	98.37	0.0163	0.0325	0.0000	0.0022	0.4851	0.0000	1.9675
1000.0	97.85	0.0215	0.0430	0.0000	0.0004	0.4881	0.0000	1.9570

TABLE C- 9 CS2 + SC2 = CO2 + 3/X SX (X=ATOMIC NO. OF DIFF. S SPECIE)

TEMP. (DEG. K)	EQUILM. CONV. (PCT)	EQUILIBRIUM DISTRIBUTION						
		CS2	SC2	S8	S6	S2	S1	CO2
300.0	100.00	0.0000	0.0000	0.3747	0.0003	0.0000	0.0000	1.0000
350.0	100.00	0.0000	0.0000	0.3735	0.0020	0.0000	0.0000	1.0000
400.0	100.00	0.0000	0.0000	0.3692	0.0078	0.0000	0.0000	1.0000
450.0	100.00	0.0000	0.0000	0.3587	0.0217	0.0000	0.0000	1.0000
500.0	100.00	0.0000	0.0000	0.3387	0.0484	0.0000	0.0000	1.0000
550.0	100.00	0.0000	0.0000	0.3073	0.0902	0.0002	0.0000	1.0000
600.0	100.00	0.0000	0.0000	0.2661	0.1448	0.0013	0.0000	1.0000
650.0	100.00	0.0000	0.0000	0.2193	0.2055	0.0063	0.0000	1.0000
700.0	100.00	0.0000	0.0000	0.1720	0.2627	0.0238	0.0000	1.0000
750.0	99.96	0.0004	0.0004	0.1273	0.3052	0.0747	0.0000	0.9996
800.0	99.91	0.0009	0.0009	0.0856	0.3180	0.2020	0.0000	0.9991
850.0	99.82	0.0018	0.0018	0.0469	0.2771	0.4785	0.0000	0.9932
900.0	99.69	0.0031	0.0031	0.0157	0.1642	0.9397	0.0000	0.9969
950.0	99.57	0.0043	0.0043	0.0023	0.0503	1.3333	0.0000	0.9957
1000.0	99.51	0.0049	0.0049	0.0002	0.0102	1.4613	0.0000	0.9951

TABLE C-10 2COS + SO2 = 2CO2 + 1/X SX (X=ATOMIC NO. OF DIFF. S SPECIE)

TEMP. (DEG. K)	EQUIL. CONV. (PCT)	EQUILIBRIUM DISTRIBUTION						
		COS	SO2	S8	S6	S2	S1	CO2
300.0	100.00	0.0000	0.0000	0.3747	0.0004	0.0000	0.0000	2.0000
350.0	100.00	0.0000	0.0000	0.3732	0.0023	0.0000	0.0000	2.0000
400.0	100.00	0.0000	0.0000	0.3683	0.0089	0.0000	0.0000	2.0000
450.0	100.00	0.0000	0.0000	0.3564	0.0248	0.0000	0.0000	2.0000
500.0	100.00	0.0000	0.0000	0.3338	0.0549	0.0000	0.0000	2.0000
550.0	99.96	0.0008	0.0004	0.2990	0.1011	0.0003	0.0000	1.9992
600.0	99.91	0.0017	0.0009	0.2542	0.1600	0.0020	0.0000	1.9983
650.0	99.79	0.0041	0.0021	0.2047	0.2229	0.0093	0.0000	1.9959
700.0	99.56	0.0087	0.0044	0.1559	0.2784	0.0345	0.0000	1.9913
750.0	99.17	0.0166	0.0083	0.1106	0.3128	0.1066	0.0000	1.9834
800.0	98.56	0.0288	0.0144	0.0691	0.3072	0.2802	0.0000	1.9712
850.0	97.73	0.0453	0.0227	0.0324	0.2369	0.6257	0.0000	1.9547
900.0	96.89	0.0622	0.0311	0.0080	0.1102	1.0906	0.0000	1.9378
950.0	96.37	0.0726	0.0363	0.0009	0.0262	1.3635	0.0000	1.9274
1000.0	96.10	0.0772	0.0390	0.0001	0.0048	1.4268	0.0000	1.9222

TABLE C-11 2H2S + SO2 = 2H2O + 1/X SX (X=ATOMIC NO. OF DIFF. S SPECIE)

TEMP. (DEG. K)	EQUILM. CONV. (PCT)	EQUILIBRIUM DISTRIBUTION						
		H2S	SO2	S8	S6	S2	S1	H2O
300.0	100.00	0.0000	0.0000	0.3747	0.0004	0.0000	0.0000	2.0000
350.0	99.95	0.0010	0.0005	0.3730	0.0023	0.0000	0.0000	1.9990
400.0	99.77	0.0046	0.0023	0.3675	0.0089	0.0000	0.0000	1.9954
450.0	99.25	0.0150	0.0075	0.3537	0.0246	0.0000	0.0000	1.9850
500.0	98.11	0.0378	0.0189	0.3273	0.0541	0.0000	0.0000	1.9622
550.0	96.02	0.0796	0.0398	0.2864	0.0981	0.0003	0.0000	1.9204
600.0	92.73	0.1454	0.0727	0.2340	0.1510	0.0020	0.0000	1.8546
650.0	88.17	0.2366	0.1183	0.1772	0.2015	0.0091	0.0000	1.7634
700.0	82.51	0.3498	0.1749	0.1238	0.2363	0.0335	0.0000	1.6502
750.0	76.17	0.4766	0.2383	0.0779	0.2433	0.1011	0.0000	1.5234
800.0	69.80	0.6040	0.3020	0.0408	0.2096	0.2550	0.0000	1.3960
850.0	64.66	0.7067	0.3534	0.0143	0.1296	0.5238	0.0000	1.2933
900.0	62.63	0.7474	0.3737	0.0024	0.0438	0.7985	0.0000	1.2526
950.0	63.66	0.7268	0.3634	0.0002	0.0089	0.9274	0.0000	1.2732
1000.0	65.53	0.6894	0.3447	0.0000	0.0017	0.9778	0.0000	1.3106

TABLE C-12 SO2 + 2CO = 2CO2 +1/X SX (X=ATOMIC NO. OF DIFF. S SPECIE)

TEMP. (DEG. K)	EQUILM. CONV. (PCT)	EQUILIBRIUM DISTRIBUTION						
		SO2	CO	S8	S6	S2	S1	CO2
300.0	100.00	0.0000	0.0000	0.1249	0.0002	0.0000	0.0000	2.0000
350.0	100.00	0.0000	0.0000	0.1243	0.0009	0.0000	0.0000	2.0000
400.0	100.00	0.0000	0.0000	0.1222	0.0038	0.0000	0.0000	2.0000
450.0	100.00	0.0000	0.0000	0.1172	0.0105	0.0000	0.0000	2.0000
500.0	100.00	0.0000	0.0000	0.1078	0.0229	0.0000	0.0000	2.0000
550.0	100.00	0.0000	0.0000	0.0119	0.1506	0.0008	0.0000	2.0000
600.0	100.00	0.0000	0.0000	0.0771	0.0634	0.0013	0.0000	2.0000
650.0	100.00	0.0000	0.0000	0.0594	0.0854	0.0062	0.0000	2.0000
700.0	99.97	0.0003	0.0006	0.0427	0.1021	0.0226	0.0000	1.9994
750.0	99.92	0.0008	0.0016	0.0277	0.1070	0.0678	0.0000	1.9984
800.0	99.81	0.0019	0.0038	0.0144	0.0912	0.1679	0.0000	1.9962
850.0	99.62	0.0038	0.0075	0.0045	0.0509	0.3277	0.0000	1.9924
900.0	99.32	0.0068	0.0136	0.0005	0.0136	0.4536	0.0000	1.9864
950.0	98.89	0.0111	0.0221	0.0000	0.0022	0.4875	0.0000	1.9779
1000.0	98.75	0.0125	0.0250	0.0000	0.0004	0.4925	0.0000	1.9750

TABLE C-13



TEMP. (DEG. K)	EQUILM. CONV. (PCT)	EQUILIBRIUM DISTRIBUTION			
		H ₂ S	CO ₂	CS ₂	H ₂ O
300.0	0.00	2.00000	1.00000	0.00000	0.00000
350.0	0.03	1.99940	0.99970	0.00030	0.00060
400.0	0.07	1.99860	0.99930	0.00070	0.00140
450.0	0.17	1.99660	0.99830	0.00170	0.00340
500.0	0.31	1.99370	0.99690	0.00310	0.00620
550.0	0.52	1.98960	0.99480	0.00520	0.01040
600.0	0.78	1.98440	0.99220	0.00780	0.01560
650.0	1.10	1.97800	0.98900	0.01100	0.02200
700.0	1.49	1.97020	0.98510	0.01490	0.02980
750.0	1.93	1.96140	0.98070	0.01930	0.03860
800.0	2.41	1.95170	0.97590	0.02410	0.04830
850.0	2.94	1.94120	0.97060	0.02940	0.05880
900.0	3.50	1.93000	0.96500	0.03500	0.07000
950.0	4.07	1.91850	0.95930	0.04070	0.08150
1000.0	4.67	1.90650	0.95330	0.04670	0.09350

TABLE C-14

H₂S + COS = H₂O + CS₂

TEMP. (DEG. K)	EQUILM. CONV. (PCT)	EQUILIBRIUM DISTRIBUTION		
		H ₂ S	COS	H ₂ O CS ₂
300.0	0.08	0.99920	0.99920	0.00080 0.00080
350.0	0.19	0.99810	0.99810	0.00190 0.00190
400.0	0.39	0.99610	0.99610	0.00390 0.00390
450.0	0.67	0.99330	0.99330	0.00670 0.00670
500.0	1.05	0.98950	0.98950	0.01050 0.01050
550.0	1.50	0.98500	0.98500	0.01500 0.01500
600.0	2.01	0.97990	0.97990	0.02010 0.02010
650.0	2.59	0.97410	0.97410	0.02590 0.02590
700.0	3.20	0.96800	0.96800	0.03200 0.03200
750.0	3.84	0.96160	0.96160	0.03840 0.03840
800.0	4.50	0.95500	0.95500	0.04500 0.04500
850.0	5.17	0.94830	0.94830	0.05170 0.05170
900.0	5.85	0.94150	0.94150	0.05850 0.05850
950.0	6.52	0.93480	0.93480	0.06520 0.06520
1000.0	7.18	0.92820	0.92820	0.07180 0.07180

TABLE C-15

H2S + CO = H2 + COS

TEMP. (DEG. K)	EQUILY. CONV. (PCT)	EQUILIBRIUM DISTRIBUTION			
		H2S	CO	H2	COS
300.0	23.76	0.76240	0.76240	0.23760	0.23760
350.0	20.62	0.79380	0.79380	0.20620	0.20620
400.0	18.62	0.91380	0.91380	0.18620	0.18620
450.0	17.29	0.82710	0.82710	0.17290	0.17290
500.0	16.38	0.83620	0.83620	0.16380	0.16380
550.0	15.74	0.84260	0.84260	0.15740	0.15740
600.0	15.29	0.84710	0.84710	0.15290	0.15290
650.0	15.00	0.85000	0.85000	0.15000	0.15000
700.0	14.75	0.85250	0.85250	0.14750	0.14750
750.0	14.60	0.85400	0.85400	0.14600	0.14600
800.0	14.50	0.85500	0.85500	0.14500	0.14500
850.0	14.44	0.85560	0.85560	0.14440	0.14440
900.0	14.40	0.85600	0.85600	0.14400	0.14400
950.0	14.39	0.85610	0.85610	0.14390	0.14390
1000.0	14.39	0.85620	0.85620	0.14380	0.14380

TABLE C-16



TEMP. (DEG. K)	EQUILM. CONV. (PCT)	EQUILIBRIUM DISTRIBUTION			
		H ₂ S	O ₂	H ₂ O	SO ₂
300.0	100.00	0.000000	0.000000	1.000000	1.000000
350.0	100.00	0.000000	0.000000	1.000000	1.000000
400.0	100.00	0.000000	0.000000	1.000000	1.000000
450.0	100.00	0.000000	0.000000	1.000000	1.000000
500.0	100.00	0.000000	0.000000	1.000000	1.000000
550.0	100.00	0.000000	0.000000	1.000000	1.000000
600.0	100.00	0.000000	0.000000	1.000000	1.000000
650.0	100.00	0.000000	0.000000	1.000000	1.000000
700.0	100.00	0.000000	0.000000	1.000000	1.000000
750.0	100.00	0.000000	0.000000	1.000000	1.000000
800.0	100.00	0.000000	0.000000	1.000000	1.000000
850.0	100.00	0.000000	0.000000	1.000000	1.000000
900.0	100.00	0.000000	0.000000	1.000000	1.000000
950.0	100.00	0.000000	0.000000	1.000000	1.000000
1000.0	100.00	0.000000	0.000000	1.000000	1.000000

TABLE C-17

$$\text{CS}_2 + 3\text{O}_2 = \text{CO}_2 + 2\text{SO}_2$$

TEMP. (DEG. K)	EQUILY. CONV. (PCT)	EQUILIBRIUM DISTRIBUTION			
		CS ₂	O ₂	CO ₂	SO ₂
300.0	100.00	0.000000	0.000000	1.000000	2.000000
350.0	100.00	0.000000	0.000000	1.000000	2.000000
400.0	100.00	0.000000	0.000000	1.000000	2.000000
450.0	100.00	0.000000	0.000000	1.000000	2.000000
500.0	100.00	0.000000	0.000000	1.000000	2.000000
550.0	100.00	0.000000	0.000000	1.000000	2.000000
600.0	100.00	0.000000	0.000000	1.000000	2.000000
650.0	100.00	0.000000	0.000000	1.000000	2.000000
700.0	100.00	0.000000	0.000000	1.000000	2.000000
750.0	100.00	0.000000	0.000000	1.000000	2.000000
800.0	100.00	0.000000	0.000000	1.000000	2.000000
850.0	100.00	0.000000	0.000000	1.000000	2.000000
900.0	100.00	0.000000	0.000000	1.000000	2.000000
950.0	100.00	0.000000	0.000000	1.000000	2.000000
1000.0	100.00	0.000000	0.000000	1.000000	2.000000

TABLE C-18



TEMP. (DEG. K)	EQUILY. CONV. (PCT)	EQUILIBRIUM DISTRIBUTION			
		COS	CO ₂	CO	SO ₂
300.0	0.00	1.000000	2.000000	0.000000	0.000000
350.0	0.00	1.000000	2.000000	0.000000	0.000000
400.0	0.00	1.000000	2.000000	0.000000	0.000000
450.0	0.00	1.000000	2.000000	0.000000	0.000000
500.0	0.00	1.000000	2.000000	0.000000	0.000000
550.0	0.00	1.000000	2.000000	0.000000	0.000000
600.0	0.00	1.000000	2.000000	0.000000	0.000000
650.0	0.03	0.999970	1.999940	0.000090	0.000030
700.0	0.07	0.999930	1.999860	0.000210	0.000070
750.0	0.16	0.999840	1.999680	0.000480	0.000160
800.0	0.30	0.999700	1.999400	0.000900	0.000300
850.0	0.57	0.999430	1.998860	0.001710	0.000570
900.0	1.00	0.999000	1.998000	0.002990	0.001000
950.0	1.68	0.998320	1.996640	0.005040	0.001680
1000.0	2.64	0.997360	1.994720	0.007900	0.002640

TABLE C-19

$$\text{COS} + 1.5 \text{ O}_2 = \text{CO}_2 + \text{SO}_2$$

TEMP. (DEG. K)	EQUIL. CONV. (PCT)	EQUILIBRIUM DISTRIBUTION		
		COS	O ₂	SO ₂
300.0	100.00	0.000000	0.000000	1.000000
350.0	100.00	0.000000	0.000000	1.000000
400.0	100.00	0.000000	0.000000	1.000000
450.0	100.00	0.000000	0.000000	1.000000
500.0	100.00	0.000000	0.000000	1.000000
550.0	100.00	0.000000	0.000000	1.000000
600.0	100.00	0.000000	0.000000	1.000000
650.0	100.00	0.000000	0.000000	1.000000
700.0	100.00	0.000000	0.000000	1.000000
750.0	100.00	0.000000	0.000000	1.000000
800.0	100.00	0.000000	0.000000	1.000000
850.0	100.00	0.000000	0.000000	1.000000
900.0	100.00	0.000000	0.000000	1.000000
950.0	100.00	0.000000	0.000000	1.000000
1000.0	100.00	0.000000	0.000000	1.000000

TABLE C-20

$H_2S + CO_2 = COS + H_2O$

TEMP. (DEG. K)	EQUIL. CONV. (PCT)	EQUILIBRIUM DISTRIBUTION			
		H ₂ S	CO ₂	COS	H ₂ O
300.0	0.00	1.00000	1.00000	0.00000	0.00000
350.0	0.00	1.00000	1.00000	0.00000	0.00000
400.0	0.55	0.99450	0.99450	0.00550	0.00550
450.0	1.05	0.98950	0.98950	0.01050	0.01050
500.0	1.64	0.98360	0.98360	0.01640	0.01640
550.0	2.40	0.97600	0.97600	0.02400	0.02400
600.0	3.29	0.96710	0.96710	0.03290	0.03290
650.0	4.37	0.95730	0.95730	0.04370	0.04370
700.0	5.34	0.94660	0.94660	0.05340	0.05340
750.0	6.47	0.93530	0.93530	0.06470	0.06470
800.0	7.62	0.92380	0.92380	0.07620	0.07620
850.0	8.80	0.91200	0.91200	0.08800	0.08800
900.0	9.99	0.90010	0.90010	0.09990	0.09990
950.0	11.16	0.88840	0.88840	0.11160	0.11160
1000.0	12.31	0.87690	0.87690	0.12310	0.12310

APPENDIX D

ILLUSTRATION OF THE CALCULATION PROCEDURE USED
TO REDUCE THE LABORATORY RAW DATA TO KINETICS
RESULTS

A step by step procedure is outlined below which indicates how a set of experimental laboratory measurements is reduced to kinetic data using the data reduction computer program listed in Appendix E-I.

Run 8 in Appendix E-I is used as an example of illustration of the calculation method. The laboratory data taken for run 8 are:

Reactor bed temperature reading	12.81 (mv)
Reactor wall temperature reading	12.80 (mv)
Feed pressure transducer reading	34.20 (chart %)
Reactor pressure transducer reading	59.20 (chart %)
Differential pressure cell reading	49.00 (chart %)
Catalyst weight	1.2352 (gm)

Chromatogram results

	Feed			Product		
	N ₂	H ₂ S	SO ₂	N ₂	H ₂ S	SO ₂
Attenuation	-11.5	9.8	10.1	-11.5	9.8	10.1
Area	82.4	176.4	173.6	82.8	101.6	99.4
Area	82.4	176.4	173.6	82.8	102.0	99.8

First of all, the subprogram in Appendix E-I calculates the compositions of feed and product streams. The calculation steps are shown below.

The actual area of each component chromatogram is calculated by using the following formula from the measured area.

$$\begin{aligned} \text{Component area} = & \text{(average measured area)} \\ & \times (21.0 - 2 \times (\text{attenuation})) \end{aligned}$$

therefore, for feed,

$$\begin{aligned} (\text{component area})_{\text{N}_2} &= ((82.4+82.4)/2) (21 - 2 \times (-11.5)) \\ &= 3625.6 \end{aligned}$$

$$\begin{aligned} (\text{component area})_{\text{H}_2\text{S}} &= ((176.4+176.4)/2) \times (21 - \\ & \quad 2 \times (9.8)) \\ &= 247.0 \end{aligned}$$

$$\begin{aligned} (\text{component area})_{\text{SO}_2} &= ((173.6 + 173.6)/2) \times (21 - \\ & \quad 2 \times (10.1)) \\ &= 138.9 \end{aligned}$$

for product,

$$\begin{aligned} (\text{component area})_{\text{N}_2} &= ((82.8 + 82.8)/2) \times (21 - \\ & \quad 2 \times (-11.5)) \\ &= 3643.2 \end{aligned}$$

$$\begin{aligned}
 (\text{component area})_{\text{H}_2\text{S}} &= ((101.6 + 102.0)/2) \times (21 - \\
 &\quad 2 \times (9.8)) \\
 &= 142.5
 \end{aligned}$$

$$\begin{aligned}
 (\text{component area})_{\text{SO}_2} &= ((99.4 + 99.8)/2) \times (21 - \\
 &\quad 2 \times (10.1)) \\
 &= 79.7
 \end{aligned}$$

From the component area the molar ratio of the component to nitrogen is calculated by using the calibration equation of :

for feed,

$$\begin{aligned}
 \text{H}_2\text{S}/\text{N}_2 \text{ molar ratio} &= -0.0298/100 + 0.4919 (247/ \\
 &\quad 3625.6) = 0.0332
 \end{aligned}$$

$$\begin{aligned}
 \text{SO}_2/\text{N}_2 \text{ molar ratio} &= 0.01775/100 + 0.43876 (138.9/ \\
 &\quad 3625) = 0.0170
 \end{aligned}$$

for product,

$$\begin{aligned}
 \text{H}_2\text{S}/\text{N}_2 \text{ molar ratio} &= -0.0298/100 + 0.4919 (142.5/ \\
 &\quad 3643.2) = 0.0189
 \end{aligned}$$

$$\begin{aligned}
 \text{SO}_2/\text{N}_2 \text{ molar ratio} &= 0.01775/100 + 0.43876 (79.7/ \\
 &\quad 3643.2) = 0.00978
 \end{aligned}$$

Since molar ratio equals to mole fraction ratio and the sum of mole fraction equals to 1, the following equations are set for feed ,

$$Y_{N_2} + Y_{H_2S} + Y_{SO_2} = 1.0$$

$$Y_{H_2S} / Y_{N_2} = 0.0332$$

$$Y_{SO_2} / Y_{N_2} = 0.0170$$

Hence the feed composition is

$$N_2 \approx 95.22 \% \text{ (molar)} \quad *$$

$$H_2S = 3.16 \% \quad *$$

$$SO_2 = 1.61 \% \quad *$$

$$\text{Feed } H_2S/SO_2 \text{ ratio} = 1.9327 \quad *$$

Product composition is not found in this way because water and various form of sulfur species are present.

The reactor bed temperature, reactor wall temperature, feed pressure and reactor pressure are calculated by the main program listed in Appendix E-I using the laboratory measured data and the following

calibration equations,

$$\begin{aligned}
 \text{Reactor bed temperature} &= 5.3155 + 18.0706 \\
 &\quad \times (\text{measured mv}) \\
 &= 5.3155 + 18.0706 \\
 &\quad \times 12.81 \\
 &= 509.96^{\circ}\text{K}
 \end{aligned}$$

$$\begin{aligned}
 \text{Reactor wall temperature} &= 6.6860 + 17.9544 \\
 &\quad \times (\text{measured mv}) \\
 &= 6.6860 + 17.9544 \\
 &\quad \times 12.80 \\
 &= 509.66^{\circ}\text{K}
 \end{aligned}$$

$$\begin{aligned}
 \text{Reaction temperature} &= (\text{reactor bed temperature} \\
 &\quad + \text{reactor wall temperature})/2 \\
 &= 509.81^{\circ}\text{K} \quad *
 \end{aligned}$$

$$\begin{aligned}
 \text{Feed pressure} &= 785.5 + 13.17 \times (\text{measured} \\
 &\quad \text{chart percent} \quad) \\
 &= 785.5 + 13.17 \times 34.2 \quad \text{mm Hg} \\
 &= 1236 \quad \text{mm Hg} \\
 &= 24.0 \quad \text{psia}
 \end{aligned}$$

$$\begin{aligned}
 \text{Reactor pressure} &= -677.6 + 25.92 \times (\text{measured} \\
 &\quad \text{chart percent} \quad) \\
 &= -677.6 + 25.92 \times 59.2 \\
 &= 857 \quad \text{mm Hg} \\
 &= 1.13 \quad \text{atm} \quad *
 \end{aligned}$$

The uncorrected total feed rate is calculated as,

$$\text{uncorrected total feed rate} = 0.9114 + 1.6747\sqrt{Y} + 0.0229Y$$

where Y is the measured chart percent

therefore,

$$\begin{aligned} \text{uncorrected total feed rate} &= 0.9114 + 1.6747 \sqrt{49} \\ &\quad + 0.0229 \times 49 \\ &= 13.76 \text{ SCFH} \end{aligned}$$

Since N_2 was used to calibrate differential pressure cell, the above uncorrected total feed rate has to be corrected. The basis of flow rate density correction has been described in Appendix A

$$FF_{\text{mix}} = FF_{N_2} \left(\rho_{N_2} / \rho_{\text{mix}} \right)^{1/2} (492/520)$$

where FF_{mix} = flow rate of mixture at 0°C , 1 atm

FF_{N_2} = flow rate of nitrogen at 60°C , 1 atm

ρ_{N_2} = density of nitrogen at 0°C , 1 atm

ρ_{mix} = density of mixture at 0°C , 1 atm

Since ideal gas law was assumed, it makes little difference whether densities are taken at 0°C or 60°F .

$$\begin{aligned}
 \rho_{N_2} &= 28/22.403 && (\text{where } 22.403 \text{ is the} \\
 &= 1.2498 \text{ gm/l} && \text{molecular volume of } N_2) \\
 \rho_{\text{mix}} &= \frac{\sum_{i=1}^3 MW_i \times y_i}{\sum_{i=1}^3 y_i v_i} \\
 &= 28.7692/22.3865 \\
 &= 1.28511
 \end{aligned}$$

where MW_i = molecular weight of component i

y_i = mole fraction of component i

v_i = molar volume of component i (litre/gm mole)

i for N_2 is 1, for H_2S is 2 and for SO_2 is 3

therefore

$$\begin{aligned}
 FF_{\text{mix}} &= 13.76 (1.2498/1.2851)^{1/2} (492/520) \\
 &= 12.85 \\
 &= FF_0
 \end{aligned}$$

The material balance was done by the subprogram

BALAN

In BALAN,

The molar feed rate of a component is taken as

$$FF_i = ((FF_0)(y_i)) / \left(\sum_{i=1}^3 y_i v_i \right) \times 28.317$$

where FF_i = molar feed rate of component i (gm mole/hr)

FF_o = volumetric mixture feed rate

at 0°C , 1 atm (ft³/hr)

y_i = mole fraction of component i

v_i = molecular volume of component i

at 0°C , 1 atm (litre/gm-mole)

28.317 = conversion factor from ft³ to litre

therefore,

$$FF_{N_2} = (12.85 \times 0.9523 / 22.3865) \times 28.317$$

$$= 16.319 \text{ gm-mole/hr} \quad *$$

$$FF_{H_2S} = (12.85 \times 28.317 \times 0.0316 / 22.3865)$$

$$= 0.548 \text{ gm-mole/hr} \quad *$$

$$FF_{SO_2} = (12.85 \times 28.317 \times 0.0161 / 22.3865)$$

$$= 0.283 \text{ gm-mole/hr} \quad *$$

It has been mentioned that nitrogen passes through the system unreacted, so

$$FP_{N_2} = FF_{N_2} = 16.319 \text{ gm-mole/hr} \quad *$$

$$FP_{H_2S} = FP_{N_2} \times (\text{molar ratio of } H_2S/N_2) \text{ of product}$$

$$= 16.319 \times 0.0189$$

$$= 0.312 \text{ gm-mole/hr} \quad *$$

$$FP_{SO_2} = 16.319 \times 0.00978 = 0.163 \text{ gm-mole/hr} \quad *$$

where FP_{N_2} etc. are product flow rate of N_2 etc.

The product rate of sulfur is calculated on the basis that all of the reacted H_2S and SO_2 go to the formation of sulfur

$$\begin{aligned}\text{FP}_{\text{S}_x} &= (\text{FF}_{\text{H}_2\text{S}} + \text{FF}_{\text{SO}_2} - \text{FP}_{\text{H}_2\text{S}} - \text{FP}_{\text{SO}_2})/X \\ &= (0.548 + 0.283 - 0.312 - 0.163) / 7.59 \\ &= 0.046 \quad \text{gm-mole/hr} \quad *\end{aligned}$$

where X is the atomic number of a sulfur species S_x . The method of arriving at $X = 7.59$ will be discussed later.

The product rate of water is calculated on the basis of the amount of H_2S and SO_2 reacted

$$\begin{aligned}\text{FP}_{\text{H}_2\text{O}} &= (2x (\text{FF}_{\text{SO}_2} - \text{FP}_{\text{SO}_2}) + (\text{FF}_{\text{H}_2\text{S}} - \text{FP}_{\text{H}_2\text{S}}))/2 \\ &= (2 \times (0.283 - 0.163) + (0.548 - 0.312))/2 \\ &= 0.24 \quad \text{gm-mole/hr} \quad *\end{aligned}$$

Now, there will be an error in the material balance due to inaccuracies in the chromatogram area measurements. This error is established by calculating the

product rate of hydrogen

$$\begin{aligned}
 FP_{H_2} &= FF_{H_2S} - FP_{H_2S} - FP_{H_2O} \\
 &= 0.548 - 0.312 - 0.24 \\
 &= -0.004
 \end{aligned}$$

*

The average molecular weight of sulfur, X, is calculated by using free energy minimization program as indicated in Appendix C. The average molecular weight is a function of the temperature (reaction temperature) and the total pressure of the sulfur species. A value of X is guessed and using it, FP_{S_x} is calculated using the product flow rates to determine its mole fraction and subsequently its partial pressure. The free energy minimization routine, given the sulfur partial pressure and temperature will calculate the average molecular weight of S based on sulfur species distribution. The latest value is compared to the last calculated and if the error exceeds 0.5%, the latest value of the average sulfur gas molecular weight is used for the next guess. The cycle continues until the error criteria is satisfied. This approach assumes that sulfur vapor is at equilibrium and the basis for this assumption has

has been described^{**}. The partial pressures of each of the species in the reactor are calculated on the basis of the product stream composition assuming that the ideal gas law applies.

$$p_i = (\text{reactor pressure}) (\text{mole fraction of component } i \text{ in reactor})$$

$$p_{N_2} = 856.8 \times (16.319/17) = 818.5 \text{ mm Hg} *$$

$$p_{H_2S} = 856.8 \times (0.312/17) = 15.6 \text{ mm Hg} *$$

$$p_{SO_2} = 856.8 \times (0.046/17) = 8.1 \text{ mm Hg} *$$

$$p_{S_x} = 856.8 \times (0.046/17) = 12.0 \text{ mm Hg} *$$

$$p_{H_2O} = 856.8 \times (0.24/17) = 2.3 \text{ mm Hg} *$$

Other data which are calculated by the computer program listed in Appendix E-I are printed out included:

$$\begin{aligned} & \text{weight of catalyst}/(\text{feed rate of } H_2S) \\ & = W/H_2S = 2.88 \text{ gm-hr}/(\text{std ft}^3) \end{aligned} *$$

$$\begin{aligned} & \text{reaction rate of } H_2S + (FF_{H_2S} - FP_{H_2S})/WC \\ & = (0.548 - 0.312) / 1.2352 \\ & = 0.1906 \text{ gm-mole/hr-gm of cat.} \end{aligned} *$$

^{**} McGregor, D.E., PhD thesis, University of Alberta, 1971

$$\begin{aligned}
 \text{reaction rate of SO}_2 &= (FF_{\text{SO}_2} - FP_{\text{SO}_2})/WC \\
 &= (0.283 - 0.163)/1.2352 \\
 &= 0.0975 \text{ gm-mole/hr-gm of cat} *
 \end{aligned}$$

$$\begin{aligned}
 \text{product H}_2\text{S/SO}_2 \text{ ratio} &= FP_{\text{H}_2\text{S}} / FP_{\text{SO}_2} \\
 &= 0.312/0.163 \\
 &= 1.9161 *
 \end{aligned}$$

$$\begin{aligned}
 \text{conversion of H}_2\text{S} (\%) &= 100 \times (FF_{\text{H}_2\text{S}} - FP_{\text{H}_2\text{S}})/FF_{\text{H}_2\text{S}} \\
 &= 100 \times (0.548 - 0.312)/0.548 \\
 &= 42.95 \% *
 \end{aligned}$$

$$\begin{aligned}
 \text{conversion of SO}_2 (\%) &= 100 \times (FF_{\text{SO}_2} - FP_{\text{SO}_2})/FF_{\text{SO}_2} \\
 &= 100 \times (0.293 - 0.163)/0.283 \\
 &= 42.45 \% *
 \end{aligned}$$

All of the foregoing numbers which are marked by an asterisk are part of the print out of the computer program. The print out was done by the subprogram OUTPT. The method of calculation for the COS/SO₂ is just the same except that the component H₂S is replaced by COS and CO₂.

APPENDIX E

LISTING OF THE LABORATORY MEASURED DATA AS
WELL AS KINETICS RESULTS

MAINLINE H2SSO

```

*****
*
*           MAINLINE H2SSO
*
* THIS PROGRAM CALCULATES THE KINETIC DATA FROM THE
* RAW PROCESS TEMPERATURES, PRESSURES, FEED AND
* PRODUCT GAS CHROMATOGRAPH PEAK AREA AND FLOW RATE
* DATA
*
*   -- INPUT DATA --
*   NRUN      - RUN NUMBER OF THE FIRST RUN
*   NCOPY     - NUMBER OF COPIES OF OUTPUT REQUIRED
*   NXXX      - TOTAL NUMBER OF RUNS
*   PREN(1)   - FEED PRESSURE RECORDER READING (PCT)
*   PREN(2)   - REACTOR PRESSURE RECORDER
*               READING (PCT)
*   PREN(3)   - D/P CELL READING (PCT)
*   TEMP(1)   - FEED TEMPERATURE (DEG. F)
*   TEMP(2)   - REACTOR TEMPERATURE (DEG. K)
*   IGCDF     - NUMBER OF FEED GAS CHROMATOGRAMS
*   IGCPD     - NUMBER OF PRODUCT GAS CHROMATOGRAMS
*   FDCR      - GAS CHROMATOGRAPH PEAK AREA OF
*               SPECIES IN FEED
*   PDCR      - GAS CHROMATOGRAPH PEAK AREA OF
*               SPECIES IN PRODUCT
*   NTL       - NUMBER OF CARDS REQUIRED TO ENTER
*               THE NAME OF THE CATALYST
*   CATNM     - CATALYST NAME
*   WC        - WEIGHT OF CATALYST
*****

```

```

DIMENSION V(3),PREN(3),CATNM(10,15),P(2,2),TEMP(2),FDC
1R(6,3),PRCR(6,3),FDCOM(7),PRCOM(7),DP(3)
DATA DP/0.91140,1.67467,0.02285/
DATA V/22403.60,22144.24,21889.30/
DATA P/785.4835,13.1717,-677.5720,25.9188/
READ (5,1) NRUN,NCOPY,NXXX
1 FORMAT (3I5)
DO 10 IRN=1,NXXX
READ (5,2) PREN(1),PREN(2),PREN(3)
2 FORMAT (3F10.5)
PREN(3)=PREN(3)**0.5
PREN(3)=DP(1)+DP(2)*PREN(3)+DP(3)*PREN(3)**2
READ (5,3) TEMP(1),TEMP(2)

```


MAINLINE H2SSO(CONTINUED)

```

3  FORMAT (2F10.5)
   READ (5,21) IGCFD
21  FORMAT (I5)
   DO 5 I=1,IGCFD
   READ (5,4) (FDCR(I,J),J=1,3)
4  FORMAT (3F10.5)
5  CONTINUE
   CALL CHROM (FDCR,FDCOM,IGCFD)
   READ (5,31) IGCPD
31  FORMAT (I5)
   DO 6 I=1,IGCPD
   READ (5,4) (PRCR(I,J),J=1,3)
6  CONTINUE
   CALL CHROM(PRCR,PRCOM,IGCPD)
C  *** DENSITY CORRECTION IN FEED FLOW RATE
   RON2=28./V(1)
   ROMIX=28./V(1)*FDCOM(1)+34./V(2)*FDCOM(2)+64./V(3)
1*FDCOM(3)
   PREN(3)=PREN(3)*(RON2/ROMIX)**0.5
   READ (5,41) NTL
41  FORMAT (I5)
   DO 8 NT=1,NTL
   READ(5,7) (CATNM(NT,K),K=1,15)
7  FORMAT (15A4)
8  CONTINUE
   READ (5,9) WC
9  FORMAT (F10.5)
   RTEMP=TEMP(2)
   PREN(1)=P(1,1)+PREN(1)*P(2,1)
   PREN(2)=P(1,2)+PREN(2)*P(2,2)
   CALL BALAN(PREN,FDCOM,PRCOM,RTEMP,WC,NRUN,NCOPY,CATNM,
1NTL)
10 NRUN=NRUN+1
   WRITE (6,50) NXXX
50  FORMAT ('1',10X,'TOTAL NUMBER OF RUNS =',I5)
   CALL EXIT
   END

```


SUBROUTINE CHROM

```

C *****
C *
C *          SUBROUTINE CHROM
C *
C * THIS PROGRAM CALCULATES THE FEED AND PRODUCT
C * COMPOSITIONS FROM THE FEED AND PRODUCT GAS
C * CHROMATOGRAPH PEAK AREAS
C *
C *****
SUBROUTINE CHROM(CR,COMP,N)
DIMENSION COMP(7),CR(6,3),ATTEN(3),CHSN2(2),CSON2(2)
DATA CHSN2/-0.02980,0.49192/
DATA CSON2/0.01775,0.43876/
DATA ATTEN/-11.5,9.8,10.1/
XN=N
DO 1 J=1,3
CR(6,J)=0.
DO 1 I=1,N
1 CR(6,J)=CR(6,J)+CR(I,J)*(21.-2.*ATTEN(J))/XN
HNRAC=CHSN2(1)/100.+CHSN2(2)*CR(6,2)/CR(6,1)
SNRAC=CSON2(1)/100.+CSON2(2)*CR(6,3)/CR(6,1)
COMP(1)=1./(1.+HNRAC+SNRAC)
COMP(2)=1.-COMP(1)-SNRAC*COMP(1)
COMP(3)=1.-COMP(1)-HNRAC*COMP(1)
RETURN
END

```


SUBROUTINE BALAN

```

C      ****
C      *
C      *          SUBROUTINE BALAN
C      *
C      * THIS PROGRAM FINDS OUT THE RATE OF REACTION AND
C      * THE MATERIAL BALANCE OF EACH SPECIE
C      *
C      ****

      SUBROUTINE BALAN(PRESS,FDCOM,PRCOM,RTEMP,WC,NRUN,NCOPY
1,CATNM,NTL,NZNG)
      DIMENSION PRCOM(7),FDCOM(7),BAL(2,7),PRESS(3),V(3)
1,CATNM(10,15)
      DATA V/22403.60,22144.24,21889.30/
      DO 10 J=1,3
10 BAL(1,J)=FDCOM(J)*PRESS(3)/V(J)*28317.016
      BAL(2,1)=BAL(1,1)
      BAL(2,2)=BAL(2,1)*(PRCOM(2)*V(1)/PRCOM(1)/V(2))
      BAL(2,3)=BAL(2,1)*(PRCOM(3)*V(1)/PRCOM(1)/V(3))
      BAL(2,4)=2.*(BAL(1,3)-BAL(2,3))
      BAL(2,5)=BAL(1,2)+BAL(1,3)-BAL(2,2)-BAL(2,3)
C      *** CALCULATE AVERAGE MOLECULAR WEIGHT OF SULFUR
      PRS=PRESS(2)/760.*BAL(2,5)/8.
22 CALL FREM(PRS,RTEMP,XS)
      PRS1=PRESS(2)/760.*BAL(2,5)/XS
      IF(ABS((PRS-PRS1)/PRS1)-0.005) 20,20,21
21 PRS=PRS1
      GO TO 22
20 BAL(2,5)=BAL(2,5)/XS
      BAL(2,6)=BAL(1,2)-BAL(2,2)-BAL(2,4)
C      *** CALCULATE REACTION RATES
      RXH2S=(BAL(1,2)-BAL(2,2))/WC
      RXSO2=(BAL(1,3)-BAL(2,3))/WC
C      *** CALCULATE FEED AND PRODUCT H2S/SO2 RATIOS
      FDRAT=BAL(1,2)/BAL(1,3)
      PRRAT=BAL(2,2)/BAL(2,3)
C      *** CALCULATE CONVERSION OF H2S AND SO2
      H2SCN=(BAL(1,2)-BAL(2,2))/BAL(1,2)*100.
      SO2CN=(BAL(1,3)-BAL(2,3))/BAL(1,3)*100.
      PRESS(3)=WC/(PRESS(3)*FDCOM(2))
C      *** CALCULATE PARTIAL PRESSURES IN REACTOR
      TOT=0.
      DO 12 J=1,5
      FDCOM(J)=FDCOM(J)*100.
12 TOT=TOT+BAL(2,J)

```


SUBROUTINE BALAN.....(CONTINUED)

```
      DO 13 J=1,5
13  PRCOM(J)=BAL(2,J)*PRESS(2)/TOT
C   *** DATA OUTPUT
      DO 100 ICOP=1,NCOPY
      CALL OUTPT(NRUN,RXH2S,RXSO2,RTEMP,PRESS,PRCOM,FDCOM,
1FDRAT,PRRAT,BAL,H2SCN,SO2CN,CATNM,WC,NTL,XS,NZNG)
100 CONTINUE
      RETURN
      END
```


SUBROUTINE OUTPT

```

C      *****
C      *
C      *              OUTPT
C      *
C      * OUTPT HAS THE SOLE FUNCTION OF WRITING OUT THE
C      * CALCULATED RESULTS ON THE LINE PRINTER
C      *
C      *****

      SUBROUTINE OUTPT (NRUN,RXH2S,RXSO2,RTEMP,PRESS,PRCOM,
1FDCOM,FDRAT,PRRAT,BAL,H2SCN,SO2CN,CATNM,WC,NTL,XS,NZNG
      DIMENSION PRESS(3),PRCOM(7),FDCOM(7),BAL(2,7),
1CATNM(10,15)
      WRITE(6,5)
5  FORMAT('1')
      WRITE(6,1) NRUN,NZNG
1  FORMAT ( 34X,'E-',I2,///10X,'RUN NUMBER',I3,/37X,'UNIT
118X,'MASS.....GRAM'//
118X,'PRESSURE.....MILLIMETERS OF MERCURY'//
118X,'TEMPERATURE.....DEGREES KELVIN'//
318X,'TIME.....HOUR' / )
      WRITE (6,50)
50 FORMAT (18X,'COMPOSITION.....MOLE PERCENT'//
118X,'VOLUME.....STANDARD CUBIC FEET'//
218X,'REACTION RATE...GM MOLES/(HR-GM OF CATALYST)'// )
      WRITE(6,3) PRESS(3)
3  FORMAT(10X,'W/FH2S (WEIGHT OF CATALYST/H2S VOLUMETRIC'
1,' FEED RATE)',2X,F6.3/)
      WRITE(6,2) RXH2S,RXSO2,RTEMP,PRESS(2)
2  FORMAT(10X,'REACTION RATE OF H2S',F7.4,5X ,
1'REACTION RATE OF SO2 ',F7.4//10X,
2 'REACTION TEMPERATURE',F7.2,5X ,
3'REACTION PRESSURE      ',F7.1/)
      WRITE(6,6) FDRAT,PRRAT,H2SCN,SO2CN
6  FORMAT(10X,'FEED H2S/SO2 RATIO  ',F7.4,5X ,
1'PRODUCT H2S/SO2 RATIO',F7.4//10X,
3'CONVERSION OF H2S      ',F7.2,5X ,
4'CONVERSION OF SO2      ',F7.2///)
      WRITE (6,55)
55 FORMAT(10X,'MOLECULAR',5X,'FEED',6X,'PARTIAL PRESSURE'
1,4X,'MATERIAL BALANCE'//11X,'SPECIE',4X,'COMPOSITION'
2,4X;'IN REACTOR',8X,'FEED      PRODUCT'//)
      WRITE(6,4) (FDCOM(J),PRCOM(J),BAL(1,J),BAL(2,J) ,
1J=1,6)
4  FORMAT (13X,'N2 ',7X,F6.2,9X,F6.1,9X,F7.3,3X,F7.3//

```


SUBROUTINE OUTPT.....(CONTINUED)

```

113X,'H2S',7X,F6.2,9X,F6.1,9X,F7.3,3X,F7.3//13X,'SO2',
27X,F6.2,9X,F6.1,9X,F7.3,3X,F7.3//13X,'H2O',7X,F6.2,9X,
3F6.1,9X,F7.3,3X,F7.3//13X,'SX ',7X,F6.2,9X,F6.1,9X,
42(F7.3,3X)//13X'H2'8X,F6.2,9X,F6.1,9X,2(F7.3,3X))
  WRITE(6,30) XS
30 FORMAT (/10X,'X=AVERAGE NUMBER OF ATOMS PER ',
1'MOLECULE =' ,F9.5/)
  DO 11 I=1,NTL
    WRITE(6,10) (CATNM(I,J),J=1,15)
10 FORMAT(10X,15A4)
11 CONTINUE
    WRITE (6,12) WC
12 FORMAT (/10X,'WEIGHT OF CATALYST =' ,F10.5,' (GRAMS)')
  RETURN
  END

```


NOTE:

The Program FREM listed in Appendix C was also used here. To avoid repetition, this program was not listed here.

MAINLINE COSSO

```

*****
*
*                               MAINLINE COSSO
*
* THIS PROGRAM CALCULATES THE KINETIC DATA FROM THE
* RAW PROCESS TEMPERATURES, PRESSURES, FEED AND
* PRODUCT GAS CHROMATOGRAPH PEAK AREA AND FLOW RATE
* DATA
*
*      -- INPUT DATA --
*
*      NRUN      - RUN NUMBER OF THE FIRST RUN
*      NCOPY     - NUMBER OF COPIES OF OUTPUT REQUIRED
*      NXXX      - TOTAL NUMBER OF RUNS
*      PREN(1)   - FEED PRESSURE RECORDER READING (PCT)
*      PREN(2)   - REACTOR PRESSURE RECORDER
*                  READING (PCT)
*      PREN(3)   - D/P CELL READING (PCT)
*      TEMP(1)   - FEED TEMPERATURE (DEG. F)
*      TEMP(2)   - REACTOR TEMPERATURE (DEG. K)
*      IGCDF     - NUMBER OF FEED GAS CHROMATOGRAMS
*      IGCDF     - NUMBER OF PRODUCT GAS CHROMATOGRAMS
*      FDCR      - GAS CHROMATOGRAPH PEAK AREA OF
*                  SPECIES IN FEED
*      PDCR      - GAS CHROMATOGRAPH PEAK AREA OF
*                  SPECIES IN PRODUCT
*      NTL       - NUMBER OF CARDS REQUIRED TO ENTER
*                  THE NAME OF THE CATALYST
*      CATNM     - CATALYST NAME
*      WC        - WEIGHT OF CATALYST
*
*****

```

```

DIMENSION V(4),PREN(3),CATNM(10,15),P(2,2),TEMP(2),
1FDCR(6,4),PRCR(6,4),FDCOM(7),PRCOM(7),DP(3)
DATA DP/0.91140,1.67467,0.02285/
DATA V/22403.60,22346.10,22399.54,21889.30/
DATA P/785.4835,13.1717,-677.5720,25.9188/
READ (5,1) NRUN,NCOPY,NXXX
1 FORMAT (3I5)
DO 10 IRN=1,NXXX
READ (5,2) PREN(1),PREN(2),PREN(3),TZZZ
2 FORMAT (4F10.5)
PREN(3)=PREN(3)**0.5
PREN(3)=DP(1)+DP(2)*PREN(3)+DP(3)*PREN(3)**2
READ (5,3) TEMP(1),TEMP(2)

```


MAINLINE COSSO(CONTINUED)

```

3  FORMAT (2F10.5)
   READ (5,21) IGCFD
21  FORMAT (I5)
   DO 5 I=1,IGCFD
   READ (5,4) (FDCR(I,J),J=1,4)
4  FORMAT (4F10.5)
5  CONTINUE
   CALL CHROM (FDCR,FDCOM,IGCFD)
   READ (5,31) IGCPD
31  FORMAT (I5)
   DO 6 I=1,IGCPD
   READ (5,4) (PRCR(I,J),J=1,4)
6  CONTINUE
   CALL CHROM(PRCR,PRCOM,IGCPD)
C  *** DENSITY CORRECTION IN FEED FLOW RATE
   RON2=28./V(1)
   ROMIX=28./V(1)*FDCOM(1)+44./V(2)*FDCOM(2)+60./V(3)*
1  FDCOM(3)+64./V(4)*FDCOM(4)
   PREN(3)=PREN(3)*(RON2/ROMIX)**0.5
   READ (5,41) NTL
41  FORMAT (I5)
   DO 8 NT=1,NTL
   READ(5,7) (CATNM(NT,K),K=1,15)
7  FORMAT (15A4)
8  CONTINUE
   READ (5,9) WC
9  FORMAT (F10.5)
   RTEMP=TEMP(2)
   PREN(1)=P(1,1)+PREN(1)*P(2,1)
   PREN(2)=P(1,2)+PREN(2)*P(2,2)
   CALL BALAN(PREN,FDCOM,PRCOM,RTEMP,WC,NRUN,NCOPY,
1  CATNM,NTL,TZZZ)
10  NRUN=NRUN+1
   WRITE (6,50) NXXX
50  FORMAT ('1',10X,'TOTAL NUMBER OF RUNS =',I5)
   CALL EXIT
   END

```


NOTE:

The Programs : CHROM, BALAN and OUTPT
were also used here. To avoid repetition,
these programs which were used earlier with
H2SS0 were not listed here.

RUN NUMBER 7 GAMMA ALUMINA- H₂S/SO₂
 THERMOCOUPLE MV READINGS FOXBORO RECORDER READINGS

12.82	12.80	12.56	34.20	59.20	72.00	1.2352
RTOR	RTOR	FLUID	FEED	RTOR	D/P	CATALYST
BED	WALL	BATH	PRESS	PRESS	CELL	WEIGHT

GAS CHROMATOGRAPH RESULTS

	FEED			PRODUCT		
	N ₂	H ₂ S	SO ₂	N ₂	H ₂ S	SO ₂
ATTENUATION	-11.5	9.8	10.1	-11.5	9.8	10.1
AREA.....	82.4	176.5	173.5	89.6	120.4	118.2
AREA.....	82.4	176.3	173.7	89.6	120.6	118.0

RUN NUMBER 8 GAMMA ALUMINA- H₂S/SO₂
 THERMOCOUPLE MV READINGS FOXBORO RECORDER READINGS

12.81	12.80	12.55	34.20	59.20	49.00	1.2352
RTOR	RTOR	FLUID	FEED	RTOR	D/P	CATALYST
BED	WALL	BATH	PRESS	PRESS	CELL	WEIGHT

GAS CHROMATOGRAPH RESULTS

	FEED			PRODUCT		
	N ₂	H ₂ S	SO ₂	N ₂	H ₂ S	SO ₂
ATTENUATION	-11.5	9.8	10.1	-11.5	9.8	10.1
AREA.....	82.4	176.4	173.6	82.8	101.6	99.4
AREA.....	82.4	176.4	173.6	82.8	102.0	99.8

RUN NUMBER 9 GAMMA ALUMINA- H₂S/SO₂
 THERMOCOUPLE MV READINGS FOXBORO RECORDER READINGS

12.83	12.80	12.55	34.20	59.20	38.80	1.2352
RCTOR	RCTOR	FLUID	FEED	RCTOR	D/P	CATALYST
BED	WALL	BATH	PRESS	PRESS	CELL	WEIGHT

GAS CHROMATOGRAPH RESULTS

	FEED			PRODUCT		
	N ₂	H ₂ S	SO ₂	N ₂	H ₂ S	SO ₂
ATTENUATION	-11.5	9.8	10.1	-11.5	9.8	10.1
AREA.....	82.4	176.6	173.4	83.8	99.6	98.1
AREA.....	82.4	176.2	173.8	83.8	99.2	98.5

RUN NUMBER 10 GAMMA ALUMINA- H₂S/SO₂
 THERMOCOUPLE MV READINGS FOXBORO RECORDER READINGS

12.81	12.80	12.57	34.20	59.20	32.20	1.2352
RCTOR	RCTOR	FLUID	FEED	RCTOR	D/P	CATALYST
BED	WALL	BATH	PRESS	PRESS	CELL	WEIGHT

GAS CHROMATOGRAPH RESULTS

	FEED			PRODUCT		
	N ₂	H ₂ S	SO ₂	N ₂	H ₂ S	SO ₂
ATTENUATION	-11.5	9.8	10.1	-11.5	9.8	10.1
AREA.....	82.4	176.4	173.6	82.5	94.8	93.9
AREA.....	82.4	176.4	173.6	82.5	94.6	93.7

RUN NUMBER 11 GAMMA ALUMINA- H₂S/SO₂
 THERMOCOUPLE MV READINGS FOXBORO RECORDER READINGS

12.83	12.79	12.56	34.20	59.20	22.00	1.2352
RTOR	RTOR	FLUID	FEED	RTOR	D/P	CATALYST
BED	WALL	BATH	PRESS	PRESS	CELL	WEIGHT

GAS CHROMATOGRAPH RESULTS

	FEED			PRODUCT		
	N ₂	H ₂ S	SO ₂	N ₂	H ₂ S	SO ₂
ATTENUATION	-11.5	9.8	10.1	-11.5	9.8	10.1
AREA.....	82.4	176.4	173.6	82.7	92.0	91.1
AREA.....	82.4	176.4	173.6	882.7	92.0	91.1

RUN NUMBER 12 GAMMA ALUMINA- H₂S/SO₂
 THERMOCOUPLE MV READINGS FOXBORO RECORDER READINGS

12.82	12.80	12.56	34.20	59.20	13.60	1.2352
RTOR	RTOR	FLUID	FEED	RTOR	D/P	CATALYST
BED	WALL	BATH	PRESS	PRESS	CELL	WEIGHT

GAS CHROMATOGRAPH RESULTS

	FEED			PRODUCT		
	N ₂	H ₂ S	SO ₂	N ₂	H ₂ S	SO ₂
ATTENUATION	-11.5	9.8	10.1	-11.5	9.8	10.1
AREA.....	82.4	176.7	173.3	82.3	86.9	86.1
AREA.....	82.4	176.1	173.9	82.3	86.9	86.1

RUN NUMBER 13 GAMMA ALUMINA- H₂S/SO₂
 THERMOCOUPLE MV READINGS FOXBORO RECORDER READINGS

12.82	12.80	12.56	34.20	59.20	3.00	1.2352
RTOR	RTOR	FLUID	FEED	RTOR	D/P	CATALYST
BED	WALL	BATH	PRESS	PRESS	CELL	WEIGHT

GAS CHROMATOGRAPH RESULTS

	FEED			PRODUCT		
	N ₂	H ₂ S	SO ₂	N ₂	H ₂ S	SO ₂
ATTENUATION	-11.5	9.8	10.1	-11.5	9.8	10.1
AREA.....	82.4	176.4	173.6	83.4	77.0	76.0
AREA.....	82.4	176.4	173.6	83.4	77.0	76.0

RUN NUMBER 14 2 PCT. DOPED GAMMA ALUMINA- H₂S/SO₂
 THERMOCOUPLE MV READINGS FOXBORO RECORDER READINGS

12.82	12.80	12.56	34.20	59.20	72.00	1.2352
RTOR	RTOR	FLUID	FEED	RTOR	D/P	CATALYST
BED	WALL	BATH	PRESS	PRESS	CELL	WEIGHT

GAS CHROMATOGRAPH RESULTS

	FEED			PRODUCT		
	N ₂	H ₂ S	SO ₂	N ₂	H ₂ S	SO ₂
ATTENUATION	-11.5	9.8	10.1	-11.5	9.8	10.1
AREA.....	84.3	177.9	173.6	82.0	95.3	94.1
AREA.....	84.3	177.9	173.6	82.0	95.5	93.9

RUN NUMBER 15 2 PCT. DOPED GAMMA ALUMINA- H₂S/SO₂
 THERMOCOUPLE MV READINGS FOXBORO RECORDER READINGS

12.83	12.79	12.58	34.20	59.20	49.00	1.2352
RTOR	RTOR	FLUID	FEED	RTOR	D/P	CATALYST
BED	WALL	BATH	PRESS	PRESS	CELL	WEIGHT

GAS CHROMATOGRAPH RESULTS

	FEED			PRODUCT		
	N ₂	H ₂ S	SO ₂	N ₂	H ₂ S	SO ₂
ATTENUATION	-11.5	9.8	10.1	-11.5	9.8	10.1
AREA.....	84.3	178.0	173.5	82.8	88.0	87.1
AREA.....	84.3	177.8	173.7	82.8	87.8	86.9

RUN NUMBER 16 2 PCT. DOPED GAMMA ALUMINA- H₂S/SO₂
 THERMOCOUPLE MV READINGS FOXBORO RECORDER READINGS

12.83	12.81	12.56	34.20	59.20	38.80	1.2352
RTOR	RTOR	FLUID	FEED	RTOR	D/P	CATALYST
BED	WALL	BATH	PRESS	PRESS	CELL	WEIGHT

GAS CHROMATOGRAPH RESULTS

	FEED			PRODUCT		
	N ₂	H ₂ S	SO ₂	N ₂	H ₂ S	SO ₂
ATTENUATION	-11.5	9.8	10.1	-11.5	9.8	10.1
AREA.....	84.3	177.4	173.1	82.0	81.0	79.9
AREA.....	84.3	178.4	174.1	82.0	81.2	80.1

RUN NUMBER 17 2 PCT. DOPED GAMMA ALUMINA- H₂S/SO₂
THERMOCOUPLE MV READINGS FOXBORO RECORDER READINGS

12.81	12.78	12.55	34.20	59.20	32.20	1.2352
RTOR	RTOR	FLUID	FEED	RTOR	D/P	CATALYST
BED	WALL	BATH	PRESS	PRESS	CELL	WEIGHT

GAS CHROMATOGRAPH RESULTS

	FEED			PRODUCT		
	N ₂	H ₂ S	SO ₂	N ₂	H ₂ S	SO ₂
ATTENUATION	-11.5	9.8	10.1	-11.5	9.8	10.1
AREA.....	84.3	178.2	173.9	82.0	76.2	75.3
AREA.....	84.3	177.6	173.3	82.0	76.2	75.3

RUN NUMBER 18 2 PCT. DOPED GAMMA ALUMINA- H₂S/SO₂
THERMOCOUPLE MV READINGS FOXBORO RECORDER READINGS

12.82	12.79	12.56	34.20	59.20	22.00	1.2352
RTOR	RTOR	FLUID	FEED	RTOR	D/P	CATALYST
BED	WALL	BATH	PRESS	PRESS	CELL	WEIGHT

GAS CHROMATOGRAPH RESULTS

	FEED			PRODUCT		
	N ₂	H ₂ S	SO ₂	N ₂	H ₂ S	SO ₂
ATTENUATION	-11.5	9.8	10.1	-11.5	9.8	10.1
AREA.....	84.3	177.0	172.7	82.4	72.0	72.1
AREA.....	84.3	178.8	174.5	82.4	72.6	72.7

RUN NUMBER 19 2 PCT. DOPED GAMMA ALUMINA- H₂S/SO₂
 THERMOCOUPLE MV READINGS FOXBORO RECORDER READINGS

12.82	12.80	12.57	34.20	59.20	13.60	1.2352
RTOR	RTOR	FLUID	FEED	RTOR	D/P	CATALYST
BED	WALL	BATH	PRESS	PRESS	CELL	WEIGHT

GAS CHROMATOGRAPH RESULTS

	FEED			PRODUCT		
	N ₂	H ₂ S	SO ₂	N ₂	H ₂ S	SO ₂
ATTENUATION	-11.5	9.8	10.1	-11.5	9.8	10.1
AREA.....	84.3	176.9	174.6	82.7	65.3	64.3
AREA.....	84.3	178.9	172.6	82.7	65.3	64.3

RUN NUMBER 20 2 PCT. DOPED GAMMA ALUMINA- H₂S/SO₂
 THERMOCOUPLE MV READINGS FOXBORO RECORDER READINGS

12.83	12.80	12.56	34.20	59.20	3.00	1.2352
RTOR	RTOR	FLUID	FEED	RTOR	D/P	CATALYST
BED	WALL	BATH	PRESS	PRESS	CELL	WEIGHT

GAS CHROMATOGRAPH RESULTS

	FEED			PRODUCT		
	N ₂	H ₂ S	SO ₂	N ₂	H ₂ S	SO ₂
ATTENUATION	-11.5	9.8	10.1	-11.5	9.8	10.1
AREA.....	84.3	177.9	173.0	83.0	55.7	55.0
AREA.....	84.3	177.9	174.2	83.0	55.5	54.8

RUN NUMBER 21 5 PCT. DOPED GAMMA ALUMINA- H₂S/SO₂
 THERMOCOUPLE MV READINGS FOXBORO RECORDER READINGS

12.83	12.80	12.56	34.20	59.20	3.00	1.2513
RTOR	RTOR	FLUID	FEED	RTOR	D/P	CATALYST
BED	WALL	BATH	PRESS	PRESS	CELL	WEIGHT

GAS CHROMATOGRAPH RESULTS

	FEED			PRODUCT		
	N ₂	H ₂ S	SO ₂	N ₂	H ₂ S	SO ₂
ATTENUATION	-11.5	9.8	10.1	-11.5	9.8	10.1
AREA.....	84.3	176.0	172.0	83.0	57.8	57.8
AREA.....	84.3	177.4	173.2	83.0	57.0	56.0

RUN NUMBER 22 5 PCT. DOPED GAMMA ALUMINA- H₂S/SO₂
 THERMOCOUPLE MV READINGS FOXBORO RECORDER READINGS

12.82	12.80	12.55	34.20	59.20	13.60	1.2515
RTOR	RTOR	FLUID	FEED	RTOR	D/P	CATALYST
BED	WALL	BATH	PRESS	PRESS	CELL	WEIGHT

GAS CHROMATOGRAPH RESULTS

	FEED			PRODUCT		
	N ₂	H ₂ S	SO ₂	N ₂	H ₂ S	SO ₂
ATTENUATION	-11.5	9.8	10.1	-11.5	9.8	10.1
AREA.....	84.3	177.7	172.6	82.7	67.3	66.2
AREA.....	84.3	175.7	172.6	82.7	67.5	66.4

RUN NUMBER 23 5 PCT. DOPED GAMMA ALUMINA- H₂S/SO₂
 THERMOCOUPLE MV READINGS FOXBORO RECORDER READINGS

12.82	12.80	12.56	34.20	59.20	22.00	1.2515
RTOR	RTOR	FLUID	FEED	RTOR	D/P	CATALYST
BED	WALL	BATH	PRESS	PRESS	CELL	WEIGHT

GAS CHROMATOGRAPH RESULTS

	FEED			PRODUCT		
	N ₂	H ₂ S	SO ₂	N ₂	H ₂ S	SO ₂
ATTENUATION	-11.5	9.8	10.1	-11.5	9.8	10.1
AREA.....	84.3	176.2	171.6	82.4	74.7	74.9
AREA.....	84.3	177.2	173.6	82.4	74.5	73.9

RUN NUMBER 24 5 PCT. DOPED GAMMA ALUMINA- H₂S/SO₂
 THERMOCOUPLE MV READINGS FOXBORO RECORDER READINGS

12.82	12.79	12.56	34.20	59.20	32.20	1.2515
RTOR	RTOR	FLUID	FEED	RTOR	D/P	CATALYST
BED	WALL	BATH	PRESS	PRESS	CELL	WEIGHT

GAS CHROMATOGRAPH RESULTS

	FEED			PRODUCT		
	N ₂	H ₂ S	SO ₂	N ₂	H ₂ S	SO ₂
ATTENUATION	-11.5	9.8	10.1	-11.5	9.8	10.1
AREA.....	84.3	176.7	172.0	82.0	78.0	76.7
AREA.....	84.3	176.7	173.2	82.0	79.2	77.9

RUN NUMBER 25 5 PCT. DOPED GAMMA ALUMINA- H₂S/SO₂
 THERMOCOUPLE MV READINGS FOXBORO RECORDER READINGS

12.83	12.79	12.56	34.20	59.20	38.80	1.2515
RECTOR	RECTOR	FLUID	FEED	RECTOR	D/P	CATALYST
BED	WALL	BATH	PRESS	PRESS	CELL	WEIGHT

GAS CHROMATOGRAPH RESULTS

	FEED			PRODUCT		
	N ₂	H ₂ S	SO ₂	N ₂	H ₂ S	SO ₂
ATTENUATION	-11.5	9.8	10.1	-11.5	9.8	10.1
AREA.....	84.3	176.7	172.6	82.0	83.7	82.0
AREA.....	84.3	176.7	172.6	82.0	83.7	82.0

RUN NUMBER 26 5 PCT. DOPED GAMMA ALUMINA- H₂S/SO₂
 THERMOCOUPLE MV READINGS FOXBORO RECORDER READINGS

12.82	12.80	12.56	34.20	59.20	49.00	1.2515
RECTOR	RECTOR	FLUID	FEED	RECTOR	D/P	CATALYST
BED	WALL	BATH	PRESS	PRESS	CELL	WEIGHT

GAS CHROMATOGRAPH RESULTS

	FEED			PRODUCT		
	N ₂	H ₂ S	SO ₂	N ₂	H ₂ S	SO ₂
ATTENUATION	-11.5	9.8	10.1	-11.5	9.8	10.1
AREA.....	84.3	176.6	171.8	82.8	89.9	89.5
AREA.....	84.3	176.8	173.4	82.8	91.5	89.7

RUN NUMBER 27 5 PCT. DOPED GAMMA ALUMINA- H₂S/SO₂
 THERMOCOUPLE MV READINGS FOXBORO RECORDER READINGS

12.83	12.78	12.55	34.20	59.20	72.00	1.2365
RTOR	RTOR	FLUID	FEED	RTOR	D/P	CATALYST
BED	WALL	BATH	PRESS	PRESS	CELL	WEIGHT

GAS CHROMATOGRAPH RESULTS

	FEED			PRODUCT		
	N ₂	H ₂ S	SO ₂	N ₂	H ₂ S	SO ₂
ATTENUATION	-11.5	9.8	10.1	-11.5	9.8	10.1
AREA.....	84.3	176.9	173.0	82.0	98.4	97.2
AREA.....	84.3	176.5	172.2	82.0	97.2	95.6

RUN NUMBER 28 BAUXITE - H₂S/SO₂
 THERMOCOUPLE MV READINGS FOXBORO RECORDER READINGS

12.81	12.79	12.56	34.20	59.20	3.00	1.2365
RTOR	RTOR	FLUID	FEED	RTOR	D/P	CATALYST
BED	WALL	BATH	PRESS	PRESS	CELL	WEIGHT

GAS CHROMATOGRAPH RESULTS

	FEED			PRODUCT		
	N ₂	H ₂ S	SO ₂	N ₂	H ₂ S	SO ₂
ATTENUATION	-11.5	9.8	10.1	-11.5	9.8	10.1
AREA.....	78.9	174.0	173.0	79.5	98.7	96.3
AREA.....	78.9	176.0	171.0	79.5	98.5	96.5

RUN NUMBER 29 BAUXITE - H₂S/SO₂
 THERMOCOUPLE MV READINGS FOXBORO RECORDER READINGS

12.82	12.79	12.55	34.20	59.20	13.60	1.2365
RTOR	RTOR	FLUID	FEED	RTOR	D/P	CATALYST
BED	WALL	BATH	PRESS	PRESS	CELL	WEIGHT

GAS CHROMATOGRAPH RESULTS

	FEED			PRODUCT		
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	N ₂	H ₂ S	SO ₂		N ₂	H ₂ S	SO ₂
ATTENUATION	-11.5	9.8	10.1		-11.5	9.8	10.1
AREA.....	78.9	175.5	172.3		79.1	109.4	107.2
AREA.....	78.9	174.5	171.7		79.1	109.0	107.0

RUN NUMBER 30 BAUXITE - H₂S/SO₂
 THERMOCOUPLE MV READINGS FOXBORO RECORDER READINGS

12.82	12.78	12.55	34.20	59.20	22.00	1.2365
RTOR	RTOR	FLUID	FEED	RTOR	D/P	CATALYST
BED	WALL	BATH	PRESS	PRESS	CELL	WEIGHT

GAS CHROMATOGRAPH RESULTS

	FEED			PRODUCT		
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	N ₂	H ₂ S	SO ₂		N ₂	H ₂ S	SO ₂
ATTENUATION	-11.5	9.8	10.1		-11.5	9.8	10.1
AREA.....	78.9	175.3	172.0		80.1	112.0	109.8
AREA.....	78.9	174.7	172.0		80.1	113.0	110.8

RUN NUMBER 31 BAUXITE - H₂S/SO₂
 THERMOCOUPLE MV READINGS FOXBORO RECORDER READINGS

12.82	12.80	12.56	34.20	59.20	32.20	1.2365
RTOR	RTOR	FLUID	FEED	RTOR	D/P	CATALYST
BED	WALL	BATH	PRESS	PRESS	CELL	WEIGHT

GAS CHROMATOGRAPH RESULTS

	FEED			PRODUCT		
	N ₂	H ₂ S	SO ₂	N ₂	H ₂ S	SO ₂
ATTENUATION	-11.5	9.8	10.1	-11.5	9.8	10.1
AREA.....	78.9	175.0	172.0	79.8	115.3	113.1
AREA.....	78.9	175.0	172.0	79.8	115.3	113.1

RUN NUMBER 32 BAUXITE - H₂S/SO₂
 THERMOCOUPLE MV READINGS FOXBORO RECORDER READINGS

12.83	12.81	12.57	34.20	59.20	38.80	1.2365
RTOR	RTOR	FLUID	FEED	RTOR	D/P	CATALYST
BED	WALL	BATH	PRESS	PRESS	CELL	WEIGHT

GAS CHROMATOGRAPH RESULTS

	FEED			PRODUCT		
	N ₂	H ₂ S	SO ₂	N ₂	H ₂ S	SO ₂
ATTENUATION	-11.5	9.8	10.1	-11.5	9.8	10.1
AREA.....	78.9	175.1	171.0	80.1	117.7	115.2
AREA.....	78.9	174.9	173.0	80.1	116.9	114.8

RUN NUMBER 33

BAUXITE - H₂S/SO₂

THERMOCOUPLE MV READINGS

FOXBORO RECORDER READINGS

12.83	12.80	12.57	34.20	59.20	49.00	1.2365
RECTOR	RECTOR	FLUID	FEED	RECTOR	D/P	CATALYST
BED	WALL	BATH	PRESS	PRESS	CELL	WEIGHT

GAS CHROMATOGRAPH RESULTS

FEED

PRODUCT

	N ₂	H ₂ S	SO ₂		N ₂	H ₂ S	SO ₂
ATTENUATION	-11.5	9.8	10.1		-11.5	9.8	10.1
AREA.....	78.9	174.9	172.0		79.8	118.9	116.1
AREA.....	78.9	175.0	172.0		79.8	118.9	116.3

RUN NUMBER 34

BAUXITE - H₂S/SO₂

THERMOCOUPLE MV READINGS

FOXBORO RECORDER READINGS

12.82	12.80	12.56	34.20	59.20	72.00	1.2365
RECTOR	RECTOR	FLUID	FEED	RECTOR	D/P	CATALYST
BED	WALL	BATH	PRESS	PRESS	CELL	WEIGHT

GAS CHROMATOGRAPH RESULTS

FEED

PRODUCT

	N ₂	H ₂ S	SO ₂		N ₂	H ₂ S	SO ₂
ATTENUATION	-11.5	9.8	10.1		-11.5	9.8	10.1
AREA.....	78.9	175.4	172.9		78.7	122.3	120.1
AREA.....	78.9	174.6	171.1		78.7	122.3	120.1

RUN NUMBER 35 2 PCT. DOPED BAUXITE - H₂S/SO₂
THERMOCOUPLE MV READINGS FOXBORO RECORDER READINGS

12.82	12.79	12.56	34.20	59.20	3.00	1.2375
RTOR	RTOR	FLUID	FEED	RTOR	D/P	CATALYST
BED	WALL	BATH	PRESS	PRESS	CELL	WEIGHT

GAS CHROMATOGRAPH RESULTS

	FEED			PRODUCT		
	N ₂	H ₂ S	SO ₂	N ₂	H ₂ S	SO ₂
ATTENUATION	-11.5	9.8	10.1	-11.5	9.8	10.1
AREA.....	79.8	177.2	173.6	79.9	80.6	79.5
AREA.....	79.8	176.8	173.2	79.9	81.2	80.1

RUN NUMBER 36 2 PCT. DOPED BAUXITE - H₂S/SO₂
THERMOCOUPLE MV READINGS FOXBORO RECORDER READINGS

12.83	12.79	12.56	34.20	59.20	13.60	1.2375
RTOR	RTOR	FLUID	FEED	RTOR	D/P	CATALYST
BED	WALL	BATH	PRESS	PRESS	CELL	WEIGHT

GAS CHROMATOGRAPH RESULTS

	FEED			PRODUCT		
	N ₂	H ₂ S	SO ₂	N ₂	H ₂ S	SO ₂
ATTENUATION	-11.5	9.8	10.1	-11.5	9.8	10.1
AREA.....	79.8	178.0	173.4	80.0	93.1	92.1
AREA.....	79.8	176.0	173.4	80.0	93.3	91.9

RUN NUMBER 37 2 PCT. DOPED BAUXITE - H₂S/SO₂
THERMOCOUPLE MV READINGS FOXBORO RECORDER READINGS

12.81	12.79	12.55	34.20	59.20	22.00	1.2375
RTOR	RTOR	FLUID	FEED	RTOR	D/P	CATALYST
BED	WALL	BATH	PRESS	PRESS	CELL	WEIGHT

GAS CHROMATOGRAPH RESULTS

	FEED			PRODUCT		
	N ₂	H ₂ S	SO ₂	N ₂	H ₂ S	SO ₂
ATTENUATION	-11.5	9.8	10.1	-11.5	9.8	10.1
AREA.....	79.8	177.6	174.4	80.3	99.0	98.1
AREA.....	79.8	176.4	172.4	80.3	99.0	97.9

RUN NUMBER 38 2 PCT. DOPED BAUXITE - H₂S/SO₂
THERMOCOUPLE MV READINGS FOXBORO RECORDER READINGS

12.82	12.80	12.55	34.20	59.20	32.20	1.2375
RTOR	RTOR	FLUID	FEED	RTOR	D/P	CATALYST
BED	WALL	BATH	PRESS	PRESS	CELL	WEIGHT

GAS CHROMATOGRAPH RESULTS

	FEED			PRODUCT		
	N ₂	H ₂ S	SO ₂	N ₂	H ₂ S	SO ₂
ATTENUATION	-11.5	9.8	10.1	-11.5	9.8	10.1
AREA.....	79.8	177.0	173.4	80.3	101.0	100.3
AREA.....	79.8	177.0	173.4	80.3	102.4	100.9

RUN NUMBER 39 2 PCT. DOPED BAUXITE - H₂S/SO₂
 THERMOCOUPLE MV READINGS FOXBORO RECORDER READINGS

12.82	12.80	12.56	34.20	59.20	38.80	1.2375
RTOR	RTOR	FLUID	FEED	RTOR	D/P	CATALYST
BED	WALL	BATH	PRESS	PRESS	CELL	WEIGHT

GAS CHROMATOGRAPH RESULTS

	FEED			PRODUCT		
	N ₂	H ₂ S	SO ₂	N ₂	H ₂ S	SO ₂
ATTENUATION	-11.5	9.8	10.1	-11.5	9.8	10.1
AREA.....	79.8	176.3	173.0	80.2	103.4	102.4
AREA.....	79.8	177.7	173.8	80.2	104.8	103.2

RUN NUMBER 40 2 PCT. DOPED BAUXITE - H₂S/SO₂
 THERMOCOUPLE MV READINGS FOXBORO RECORDER READINGS

12.83	1208.00	12.56	34.20	59.20	49.00	1.2375
RTOR	RTOR	FLUID	FEED	RTOR	D/P	CATALYST
BED	WALL	BATH	PRESS	PRESS	CELL	WEIGHT

GAS CHROMATOGRAPH RESULTS

	FEED			PRODUCT		
	N ₂	H ₂ S	SO ₂	N ₂	H ₂ S	SO ₂
ATTENUATION	-11.5	9.8	10.1	-11.5	9.8	10.1
AREA.....	79.8	176.9	173.3	81.2	111.6	110.1
AREA.....	79.8	177.1	173.5	81.2	111.8	110.3

RUN NUMBER 41 2 PCT. DOPED BAUXITE - H₂S/SO₂
 THERMOCOUPLE MV READINGS FOXBORO RECORDER READINGS

12.83	12.80	12.57	34.20	59.20	72.00	1.2335
RTOR	RTOR	FLUID	FEED	RTOR	D/P	CATALYST
BED	WALL	BATH	PRESS	PRESS	CELL	WEIGHT

GAS CHROMATOGRAPH RESULTS

	FEED			PRODUCT		
	N ₂	H ₂ S	SO ₂	N ₂	H ₂ S	SO ₂
ATTENUATION	-11.5	9.8	10.1	-11.5	9.8	10.1
AREA.....	79.8	177.8	173.4	81.8	120.3	118.9
AREA.....	79.8	176.2	173.4	81.8	119.7	118.9

RUN NUMBER 42 H-Y ZEOLITE - H₂S/SO₂
 THERMOCOUPLE MV READINGS FOXBORO RECORDER READINGS

12.81	12.80	12.55	34.20	59.20	3.00	1.2335
RTOR	RTOR	FLUID	FEED	RTOR	D/P	CATALYST
BED	WALL	BATH	PRESS	PRESS	CELL	WEIGHT

GAS CHROMATOGRAPH RESULTS

	FEED			PRODUCT		
	N ₂	H ₂ S	SO ₂	N ₂	H ₂ S	SO ₂
ATTENUATION	-11.5	9.8	10.1	-11.5	9.8	10.1
AREA.....	82.4	170.0	163.9	82.2	129.3	125.9
AREA.....	82.4	170.6	163.9	82.2	129.9	126.5

RUN NUMBER 43 H-Y ZEOLITE - H₂S/SO₂
 THERMOCOUPLE MV READINGS FOXBORO RECORDER READINGS

12.82	12.80	12.57	34.20	59.20	13.60	1.2335
RTOR	RTOR	FLUID	FEED	RTOR	D/P	CATALYST
BED	WALL	BATH	PRESS	PRESS	CELL	WEIGHT

GAS CHROMATOGRAPH RESULTS

	FEED			PRODUCT		
	N ₂	H ₂ S	SO ₂	N ₂	H ₂ S	SO ₂
ATTENUATION	-11.5	9.8	10.1	-11.5	9.8	10.1
AREA.....	82.4	168.4	164.2	81.7	139.0	135.5
AREA.....	82.4	168.8	164.6	81.7	139.4	135.9

RUN NUMBER 44 H-Y ZEOLITE - H₂S/SO₂
 THERMOCOUPLE MV READINGS FOXBORO RECORDER READINGS

12.83	12.79	12.56	34.20	59.20	22.00	1.2335
RTOR	RTOR	FLUID	FEED	RTOR	D/P	CATALYST
BED	WALL	BATH	PRESS	PRESS	CELL	WEIGHT

GAS CHROMATOGRAPH RESULTS

	FEED			PRODUCT		
	N ₂	H ₂ S	SO ₂	N ₂	H ₂ S	SO ₂
ATTENUATION	-11.5	9.8	10.1	-11.5	9.8	10.1
AREA.....	82.4	172.0	165.4	81.6	146.9	145.1
AREA.....	82.4	172.4	165.4	81.6	146.9	145.1

RUN NUMBER 45 H-Y ZEOLITE - H₂S/SO₂
 THERMOCOUPLE MV READINGS FOXBORO RECORDER READINGS

12.82	12.80	12.56	34.20	59.20	32.20	1.2335
RTOR	RTOR	FLUID	FEED	RTOR	D/P	CATALYST
BED	WALL	BATH	PRESS	PRESS	CELL	WEIGHT

GAS CHROMATOGRAPH RESULTS

	FEED			PRODUCT		
	N ₂	H ₂ S	SO ₂	N ₂	H ₂ S	SO ₂
ATTENUATION	-11.5	9.8	10.1	-11.5	9.8	10.1
AREA.....	82.4	171.7	165.9	81.6	150.9	144.1
AREA.....	82.4	172.7	164.9	81.6	149.9	145.1

RUN NUMBER 46 H-Y ZEOLITE - H₂S/SO₂
 THERMOCOUPLE MV READINGS FOXBORO RECORDER READINGS

12.82	12.80	12.56	34.20	59.20	38.80	1.2335
RTOR	RTOR	FLUID	FEED	RTOR	D/P	CATALYST
BED	WALL	BATH	PRESS	PRESS	CELL	WEIGHT

GAS CHROMATOGRAPH RESULTS

	FEED			PRODUCT		
	N ₂	H ₂ S	SO ₂	N ₂	H ₂ S	SO ₂
ATTENUATION	-11.5	9.8	10.1	-11.5	9.8	10.1
AREA.....	82.4	172.2	164.4	81.6	152.0	148.2
AREA.....	82.4	172.2	166.4	81.6	152.2	148.4

RUN NUMBER 47 H-Y ZEOLITE - H₂S/SO₂
 THERMOCOUPLE MV READINGS FOXBORO RECORDER READINGS

12.83	12.79	12.55	34.20	59.20	49.00	1.2335
RTOR	RTOR	FLUID	FEED	RTOR	D/P	CATALYST
BED	WALL	BATH	PRESS	PRESS	CELL	WEIGHT

GAS CHROMATOGRAPH RESULTS

	FEED			PRODUCT		
	N ₂	H ₂ S	SO ₂	N ₂	H ₂ S	SO ₂
ATTENUATION	-11.5	9.8	10.1	-11.5	9.8	10.1
AREA.....	82.4	171.2	165.3	81.4	153.0	148.3
AREA.....	82.4	173.2	165.5	81.4	153.6	148.9

RUN NUMBER 48 H-Y ZEOLITE - H₂S/SO₂
 THERMOCOUPLE MV READINGS FOXBORO RECORDER READINGS

12.83	12.80	12.56	34.20	59.20	72.00	1.2335
RTOR	RTOR	FLUID	FEED	RTOR	D/P	CATALYST
BED	WALL	BATH	PRESS	PRESS	CELL	WEIGHT

GAS CHROMATOGRAPH RESULTS

	FEED			PRODUCT		
	N ₂	H ₂ S	SO ₂	N ₂	H ₂ S	SO ₂
ATTENUATION	-11.5	9.8	10.1	-11.5	9.8	10.1
AREA.....	82.4	172.2	165.4	81.6	155.6	152.6
AREA.....	82.4	172.2	165.4	81.6	157.6	153.6

RUN NUMBER 49 NA-Y ZEOLITE - H₂S/SO₂
 THERMOCOUPLE MV READINGS FOXBORO RECORDER READINGS

12.82	12.80	12.56	34.20	59.20	3.00	1.2367
RTOR	RTOR	FLUID	FEED	RTOR	D/P	CATALYST
BED	WALL	BATH	PRESS	PRESS	CELL	WEIGHT

GAS CHROMATOGRAPH RESULTS

	FEED			PRODUCT		
	N ₂	H ₂ S	SO ₂	N ₂	H ₂ S	SO ₂
ATTENUATION	-11.5	9.8	10.1	-11.5	9.8	10.1
AREA.....	81.2	169.0	163.0	80.4	126.1	123.8
AREA.....	81.2	170.0	163.2	80.4	125.1	123.6

RUN NUMBER 50 NA-Y ZEOLITE - H₂S/SO₂
 THERMOCOUPLE MV READINGS FOXBORO RECORDER READINGS

12.82	12.80	12.55	34.20	59.20	13.60	1.2367
RTOR	RTOR	FLUID	FEED	RTOR	D/P	CATALYST
BED	WALL	BATH	PRESS	PRESS	CELL	WEIGHT

GAS CHROMATOGRAPH RESULTS

	FEED			PRODUCT		
	N ₂	H ₂ S	SO ₂	N ₂	H ₂ S	SO ₂
ATTENUATION	-11.5	9.8	10.1	-11.5	9.8	10.1
AREA.....	81.2	169.4	163.0	79.9	133.4	129.7
AREA.....	81.2	169.6	163.2	79.9	133.6	129.9

RUN NUMBER 51 NA-Y ZEOLITE - H₂S/SO₂
 THERMOCOUPLE MV READINGS FOXBORO RECORDER READINGS

12.84	12.78	12.55	34.20	59.20	22.00	1.2367
RTOR	RTOR	FLUID	FEED	RTOR	D/P	CATALYST
BED	WALL	BATH	PRESS	PRESS	CELL	WEIGHT

GAS CHROMATOGRAPH RESULTS

	FEED			PRODUCT		
	N ₂	H ₂ S	SO ₂	N ₂	H ₂ S	SO ₂
ATTENUATION	-11.5	9.8	10.1	-11.5	9.8	10.1
AREA.....	81.2	169.8	163.4	80.5	137.7	134.0
AREA.....	81.2	169.2	162.8	80.5	137.7	133.4

RUN NUMBER 52 NA-Y ZEOLITE - H₂S/SO₂
 THERMOCOUPLE MV READINGS FOXBORO RECORDER READINGS

12.83	12.78	12.56	34.20	59.20	32.20	1.2367
RTOR	RTOR	FLUID	FEED	RTOR	D/P	CATALYST
BED	WALL	BATH	PRESS	PRESS	CELL	WEIGHT

GAS CHROMATOGRAPH RESULTS

	FEED			PRODUCT		
	N ₂	H ₂ S	SO ₂	N ₂	H ₂ S	SO ₂
ATTENUATION	-11.5	9.8	10.1	-11.5	9.8	10.1
AREA.....	81.0	172.7	167.1	79.9	144.0	139.1
AREA.....	81.0	172.7	165.1	79.9	144.0	140.1

RUN NUMBER 53 NA-Y ZEOLITE - H₂S/SO₂
 THERMOCOUPLE MV READINGS FOXBORO RECORDER READINGS

12.83	12.80	12.57	34.20	59.20	38.80	1.2367
RECTOR	RECTOR	FLUID	FEED	RECTOR	D/P	CATALYST
BED	WALL	BATH	PRESS	PRESS	CELL	WEIGHT

GAS CHROMATOGRAPH RESULTS

	FEED			PRODUCT		
	N ₂	H ₂ S	SO ₂	N ₂	H ₂ S	SO ₂
ATTENUATION	-11.5	9.8	10.1	-11.5	9.8	10.1
AREA.....	81.0	172.0	165.4	80.0	145.6	141.1
AREA.....	81.0	173.4	166.8	80.0	145.4	140.8

RUN NUMBER 54 NA-Y ZEOLITE - H₂S/SO₂
 THERMOCOUPLE MV READINGS FOXBORO RECORDER READINGS

12.82	12.80	12.57	34.20	59.20	49.00	1.2367
RECTOR	RECTOR	FLUID	FEED	RECTOR	D/P	CATALYST
BED	WALL	BATH	PRESS	PRESS	CELL	WEIGHT

GAS CHROMATOGRAPH RESULTS

	FEED			PRODUCT		
	N ₂	H ₂ S	SO ₂	N ₂	H ₂ S	SO ₂
ATTENUATION	-11.5	9.8	10.1	-11.5	9.8	10.1
AREA.....	81.0	173.2	166.1	79.2	145.8	143.4
AREA.....	81.0	172.2	166.1	79.2	145.8	140.3

RUN NUMBER 55 NA-Y ZEOLITE - H₂S/SO₂
 THERMOCOUPLE MV READINGS FOXBORO RECORDER READINGS

12.82	12.80	12.56	34.20	59.20	72.00	1.2367
RECTOR	RECTOR	FLUID	FEED	RECTOR	D/P	CATALYST
BED	WALL	BATH	PRESS	PRESS	CELL	WEIGHT

GAS CHROMATOGRAPH RESULTS

	FEED			PRODUCT		
	N ₂	H ₂ S	SO ₂	N ₂	H ₂ S	SO ₂

ATTENUATION	-11.5	9.8	10.1	-11.5	9.8	10.1
AREA.....	81.0	172.3	166.5	79.1	151.6	146.3
AREA.....	81.0	173.1	165.7	79.1	151.6	146.3

RUN NUMBER 4 6.0 MIN. AFTER REACTANTS INTRODUCED

THERMOCOUPLE MV READINGS FOXBORO RECORDER READINGS

13.55	13.50	13.41	34.20	59.20	2.30	2.6842
RTOR	RTOR	FLUID	FEED	RTOR	D/P	CATALYST
BED	WALL	BATH	PRESS	PRESS	CELL	WEIGHT

GAS CHROMATOGRAPH RESULTS

	FEED			PRODUCT		
	ATTENUATION	AREA	AREA	ATTENUATION	AREA	AREA
N2.....	-9.0	87.0	87.0	-9.0	87.4	87.4
CO2.....	9.8	13.0	13.0	9.8	124.3	124.5
COS.....	9.4	127.5	127.7	9.4	56.5	56.3
SO2.....	10.1	204.2	204.4	10.1	88.7	88.5

RUN NUMBER 4 24.0 MIN. AFTER REACTANTS INTRODUCED

THERMOCOUPLE MV READINGS FOXBORO RECORDER READINGS

13.54	13.52	13.40	34.20	59.20	2.30	2.6842
RTOR	RTOR	FLUID	FEED	RTOR	D/P	CATALYST
BED	WALL	BATH	PRESS	PRESS	CELL	WEIGHT

GAS CHROMATOGRAPH RESULTS

	FEED			PRODUCT		
	ATTENUATION	AREA	AREA	ATTENUATION	AREA	AREA
N2.....	-9.0	87.0	87.0	-9.0	88.3	59.0
CO2.....	9.8	13.0	13.0	9.8	59.4	99.6
COS.....	9.4	127.8	127.4	9.4	99.2	157.8
SO2.....	10.1	204.1	204.5	10.1	158.2	0.0

RUN NUMBER 4 30.0 MIN. AFTER REACTANTS INTRODUCED

THERMOCOUPLE MV READINGS FOXBORO RECORDER READINGS

13.54	13.53	13.42	34.20	59.20	2.30	2.6842
RTOR	RTOR	FLUID	FEED	RTOR	D/P	CATALYST
BED	WALL	BATH	PRESS	PRESS	CELL	WEIGHT

GAS CHROMATOGRAPH RESULTS

FEED

PRODUCT

	ATTENUATION	AREA	AREA	ATTENUATION	AREA	AREA
N2.....	-9.0	87.0	87.0	-9.0	88.3	88.3
CO2.....	9.8	13.0	13.0	9.8	45.0	44.8
COS.....	9.4	127.7	127.5	9.4	109.1	108.7
SO2.....	10.1	204.5	204.1	10.1	174.0	173.7

RUN NUMBER 4 36.0 MIN. AFTER REACTANTS INTRODUCED

THERMOCOUPLE MV READINGS FOXBORO RECORDER READINGS

13.56	13.50	13.42	34.20	59.20	2.30	2.6842
RTOR	RTOR	FLUID	FEED	RTOR	D/P	CATALYST
BED	WALL	BATH	PRESS	PRESS	CELL	WEIGHT

GAS CHROMATOGRAPH RESULTS

FEED

PRODUCT

	ATTENUATION	AREA	AREA	ATTENUATION	AREA	AREA
N2.....	-9.0	87.0	87.0	-9.0	88.0	88.0
CO2.....	9.8	13.0	13.0	9.8	36.2	36.6
COS.....	9.4	127.3	127.9	9.4	115.4	115.4
SO2.....	10.1	204.3	204.3	10.1	184.5	184.7

RUN NUMBER 4 54.0 MIN. AFTER REACTANTS INTRODUCED

THERMOCOUPLE MV READINGS FOXBORO RECORDER READINGS

13.55	13.53	13.41	34.20	59.20	2.30	2.6842
RTOR	RTOR	FLUID	FEED	RTOR	D/P	CATALYST
BED	WALL	BATH	PRESS	PRESS	CELL	WEIGHT

GAS CHROMATOGRAPH RESULTS

	FEED			PRODUCT		
	ATTENUATION	AREA	AREA	ATTENUATION	AREA	AREA
N2.....	-9.0	87.0	87.0	-9.0	88.0	88.0
CO2.....	9.8	13.0	13.0	9.8	19.1	18.5
COS.....	9.4	127.7	127.5	9.4	125.5	126.3
SO2.....	10.1	204.5	204.1	10.1	200.9	201.9

RUN NUMBER 4 60.0 MIN. AFTER REACTANTS INTRODUCED

THERMOCOUPLE MV READINGS FOXBORO RECORDER READINGS

13.55	13.52	13.41	34.20	59.20	2.30	2.6842
RTOR	RTOR	FLUID	FEED	RTOR	D/P	CATALYST
BED	WALL	BATH	PRESS	PRESS	CELL	WEIGHT

GAS CHROMATOGRAPH RESULTS

	FEED			PRODUCT		
	ATTENUATION	AREA	AREA	ATTENUATION	AREA	AREA
N2.....	-9.0	87.0	87.0	-9.0	88.3	88.3
CO2.....	9.8	13.0	13.0	9.8	17.1	17.1
COS.....	9.4	127.8	127.4	9.4	127.2	127.2
SO2.....	10.1	204.1	204.5	10.1	203.9	203.9

RUN NUMBER 4 66.0 MIN. AFTER REACTANTS INTRODUCED

THERMOCOUPLE MV READINGS FOXBORO RECORDER READINGS

13.54	13.53	13.42	34.20	59.20	2.30	4.8874
RTOR	RTOR	FLUID	FEED	RTOR	D/P	CATALYST
BED	WALL	BATH	PRESS	PRESS	CELL	WEIGHT

GAS CHROMATOGRAPH RESULTS

FEED			PRODUCT			
	ATTENUATION	AREA	AREA	ATTENUATION	AREA	AREA
N2.....	-9.0	87.0	87.0	-9.0	88.3	88.3
CO2.....	9.8	13.0	13.0	9.8	17.1	17.1
COS.....	9.4	127.6	127.6	9.4	127.4	127.4
SO2.....	10.1	204.3	204.3	10.1	204.1	204.1

RUN NUMBER 5 6.0 MIN. AFTER REACTANTS INTRODUCED

THERMOCOUPLE MV READINGS FOXBORO RECORDER READINGS

15.49	15.45	15.30	34.20	59.20	5.20	4.8874
RTOR	RTOR	FLUID	FEED	RTOR	D/P	CATALYST
BED	WALL	BATH	PRESS	PRESS	CELL	WEIGHT

GAS CHROMATOGRAPH RESULTS

FEED			PRODUCT			
	ATTENUATION	AREA	AREA	ATTENUATION	AREA	AREA
N2.....	-9.0	92.5	92.5	-9.0	93.0	93.0
CO2.....	9.8	14.0	14.0	9.8	120.4	120.8
COS.....	9.4	116.1	115.5	9.4	45.1	45.1
SO2.....	10.1	188.9	188.9	10.1	71.3	71.1

RUN NUMBER 5 24.0 MIN. AFTER REACTANTS INTRODUCED

THERMOCOUPLE MV READINGS FOXBORO RECORDER READINGS

15.48	15.46	15.29	34.20	59.20	5.20	4.8874
RTOR	RTOR	FLUID	FEED	RTOR	D/P	CATALYST
BED	WALL	BATH	PRESS	PRESS	CELL	WEIGHT

GAS CHROMATOGRAPH RESULTS

	FEED			PRODUCT		
	ATTENUATION	AREA	AREA	ATTENUATION	AREA	AREA
N2.....	-9.0	92.5	92.5	-9.0	91.7	91.7
CO2.....	9.8	14.0	14.0	9.8	64.5	64.3
COS.....	9.4	115.6	116.0	9.4	80.1	79.7
SO2.....	10.1	188.7	189.1	10.1	130.5	129.9

RUN NUMBER 5 42.0 MIN. AFTER REACTANTS INTRODUCED

THERMOCOUPLE MV READINGS FOXBORO RECORDER READINGS

15.48	15.45	15.29	34.20	59.20	5.20	4.8874
RTOR	RTOR	FLUID	FEED	RTOR	D/P	CATALYST
BED	WALL	BATH	PRESS	PRESS	CELL	WEIGHT

GAS CHROMATOGRAPH RESULTS

	FEED			PRODUCT		
	ATTENUATION	AREA	AREA	ATTENUATION	AREA	AREA
N2.....	-9.0	92.5	92.5	-9.0	91.2	91.2
CO2.....	9.8	14.0	14.0	9.8	30.6	30.6
COS.....	9.4	115.4	116.2	9.4	103.0	102.6
SO2.....	10.1	188.8	189.0	10.1	167.8	167.4

RUN NUMBER 5 54.0 MIN. AFTER REACTANTS INTRODUCED

THERMOCOUPLE MV READINGS FOXBORO RECORDER READINGS

15.49	15.47	15.30	34.20	59.20	5.20	4.8874
RTOR	RTOR	FLUID	FEED	RTOR	D/P	CATALYST
BED	WALL	BATH	PRESS	PRESS	CELL	WEIGHT

GAS CHROMATOGRAPH RESULTS

FEED

PRODUCT

	ATTENUATION	AREA	AREA	ATTENUATION	AREA	AREA
N2.....	-9.0	92.5	92.5	-9.0	91.6	91.6
CO2.....	9.8	14.0	14.0	9.8	21.6	21.6
COS.....	9.4	115.8	115.8	9.4	109.6	109.4
SO2.....	10.1	188.6	189.2	10.1	178.6	178.4

RUN NUMBER 5 83.0 MIN. AFTER REACTANTS INTRODUCED

THERMOCOUPLE MV READINGS FOXBORO RECORDER READINGS

15.48	15.46	15.30	34.20	59.20	5.20	4.8874
RTOR	RTOR	FLUID	FEED	RTOR	D/P	CATALYST
BED	WALL	BATH	PRESS	PRESS	CELL	WEIGHT

GAS CHROMATOGRAPH RESULTS

FEED

PRODUCT

	ATTENUATION	AREA	AREA	ATTENUATION	AREA	AREA
N2.....	-9.0	92.5	92.5	-9.0	91.6	91.6
CO2.....	9.8	14.0	14.0	9.8	16.5	16.5
COS.....	9.4	115.5	116.1	9.4	112.8	113.0
SO2.....	10.1	189.4	188.4	10.1	184.1	183.9

RUN NUMBER 5 96.0 MIN. AFTER REACTANTS INTRODUCED

THERMOCOUPLE MV READINGS FOXBORO RECORDER READINGS

15.49	15.45	15.29	34.20	59.20	5.20	1.2442
RTOR	RTOR	FLUID	FEED	RTOR	D/P	CATALYST
BED	WALL	BATH	PRESS	PRESS	CELL	WEIGHT

GAS CHROMATOGRAPH RESULTS

FEED

PRODUCT

	ATTENUATION	AREA	AREA	ATTENUATION	AREA	AREA
N2.....	-9.0	92.5	92.5	-9.0	91.6	91.6
CO2.....	9.8	14.0	14.0	9.8	16.5	16.5
COS.....	9.4	115.7	115.9	9.4	114.0	114.0
SO2.....	10.1	188.8	189.0	10.1	185.1	185.1

RUN NUMBER 6 12.0 MIN. AFTER REACTANTS INTRODUCED

THERMOCOUPLE MV READINGS FOXBORO RECORDER READINGS

12.82	12.80	12.56	34.20	59.20	1.70	1.2442
RTOR	RTOR	FLUID	FEED	RTOR	D/P	CATALYST
BED	WALL	BATH	PRESS	PRESS	CELL	WEIGHT

GAS CHROMATOGRAPH RESULTS

FEED

PRODUCT

	ATTENUATION	AREA	AREA	ATTENUATION	AREA	AREA
N2.....	-9.0	92.5	92.5	-9.0	92.5	92.5
CO2.....	9.8	14.0	14.0	9.8	14.0	14.0
COS.....	9.4	115.8	115.8	9.4	115.6	115.6
SO2.....	10.1	188.9	188.9	10.1	188.8	188.8

RUN NUMBER 6 24.0 MIN. AFTER REACTANTS INTRODUCED

THERMOCOUPLE MV READINGS FOXBORO RECORDER READINGS

12.82	12.80	12.56	34.20	59.20	1.70	1.2442
RECTOR	RECTOR	FLUID	FEED	RECTOR	D/P	CATALYST
BED	WALL	PATH	PRESS	PRESS	CELL	WEIGHT

GAS CHROMATOGRAPH RESULTS

FEED	PRODUCT
1	1
2	2
3	3
4	4
5	5
6	6
7	7
8	8
9	9
10	10
11	11
12	12
13	13
14	14
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90	90
91	91
92	92
93	93
94	94
95	95
96	96
97	97
98	98
99	99
100	100

	ATTENUATION	AREA	AREA	ATTENUATION	AREA	AREA
N2.....	-9.0	92.5	92.5	-9.0	92.5	92.5
CO2.....	9.8	14.0	14.0	9.8	14.0	14.0
COS.....	9.4	115.8	115.8	9.4	116.0	115.8
SO2.....	10.1	188.9	188.9	10.1	189.0	189.0

RUN NUMBER 6 30.0 MIN. AFTER REACTANTS INTRODUCED

THERMOCOUPLE MV READINGS FOXBORO RECORDER READINGS

12.82	12.80	12.56	34.20	59.20	1.70	1.2442
RECTOR	RECTOR	FLUID	FEED	RECTOR	D/P	CATALYST
BED	WALL	BATH	PRESS	PRESS	CELL	WEIGHT

GAS CHROMATOGRAPH RESULTS

FEED	PRODUCT
1	1
2	2
3	3
4	4
5	5
6	6
7	7
8	8
9	9
10	10
11	11
12	12
13	13
14	14
15	15
16	16
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18	18
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85	85
86	86
87	87
88	88
89	89
90	90
91	91
92	92
93	93
94	94
95	95
96	96
97	97
98	98
99	99
100	100

	ATTENUATION	AREA	AREA	ATTENUATION	AREA	AREA
N2.....	-9.0	92.5	92.5	-9.0	92.5	92.5
CO2.....	9.8	14.0	14.0	9.8	14.0	14.0
COS.....	9.4	115.8	115.8	9.4	115.8	115.8
SO2.....	10.1	188.9	188.9	10.1	188.9	188.9

RUN NUMBER 7

UNITS

MASS.....GRAM

PRESSURE.....MILLIMETERS OF MERCURY

TEMPERATURE.....DEGREES KELVIN

TIME.....HOUR

COMPOSITION.....MOLE PERCENT

VOLUME.....STANDARD CUBIC FEET

REACTION RATE...GM MOLES/(HR-GM OF CATALYST)

W/FH₂S (WEIGHT OF CATALYST/H₂S VOLUMETRIC FEED RATE) 2.363REACTION RATE OF H₂S 0.2029 REACTION RATE OF SO₂ 0.1037

REACTION TEMPERATURE 510.00 REACTION PRESSURE 856.8

FEED H₂S/SO₂ RATIO 1.9327 PRODUCT H₂S/SO₂ RATIO 1.9184CONVERSION OF H₂S 37.51 CONVERSION OF SO₂ 37.04

MOLECULAR	FEED	PARTIAL PRESSURE	MATERIAL BALANCE	
SPECIE	COMPOSITION	IN REACTOR	FEED	PRODUCT
N ₂	95.22	818.1	19.893	19.893
H ₂ S	3.16	17.1	0.668	0.417
SO ₂	1.61	8.9	0.345	0.217
H ₂ O	0.00	10.5	0.000	0.256
SX	0.00	2.0	0.000	0.049
H ₂	0.00	0.0	0.000	-0.005

X=AVERAGE NUMBER OF ATOMS PER MOLECULE = 7.59388

GAMMA ALUMINA

WEIGHT OF CATALYST = 1.23520 (GRAMS)

RUN NUMBER 8

UNITS

MASS.....GRAM

PRESSURE.....MILLIMETERS OF MERCURY

TEMPERATURE.....DEGREES KELVIN

TIME.....HOUR

COMPOSITION.....MOLE PERCENT

VOLUME.....STANDARD CUBIC FEET

REACTION RATE...GM MOLES/(HR-GM OF CATALYST)

W/FH ₂ S (WEIGHT OF CATALYST/H ₂ S VOLUMETRIC FEED RATE)	2.880
REACTION RATE OF H ₂ S 0.1906	REACTION RATE OF SO ₂ 0.0975
REACTION TEMPERATURE 510.00	REACTION PRESSURE 856.8
FEED H ₂ S/SO ₂ RATIO 1.9327	PRODUCT H ₂ S/SO ₂ RATIO 1.9161
CONVERSION OF H ₂ S 42.95	CONVERSION OF SO ₂ 42.45

MOLECULAR SPECIE	FEED COMPOSITION	PARTIAL PRESSURE IN REACTOR	MATERIAL BALANCE	
			FEED	PRODUCT
N ₂	95.22	818.5	16.319	16.319
H ₂ S	3.16	15.6	0.548	0.312
SO ₂	1.61	8.1	0.283	0.163
H ₂ O	0.00	12.0	0.000	0.240
SX	0.00	2.3	0.000	0.046
H ₂	0.00	0.0	0.000	-0.005

X=AVERAGE NUMBER OF ATOMS PER MOLECULE = 7.58854

GAMMA ALUMINA

WEIGHT OF CATALYST = 1.23520 (GRAMS)

RUN NUMBER 9

UNITS

MASS.....GRAM

PRESSURE.....MILLIMETERS OF MERCURY

TEMPERATURE.....DEGREES KELVIN

TIME.....HOUR

COMPOSITION.....MOLE PERCENT

VOLUME.....STANDARD CUBIC FEET

REACTION RATE...GM MOLES/(HR-GM OF CATALYST)

W/FH₂S (WEIGHT OF CATALYST/H₂S VOLUMETRIC FEED RATE) 3.239REACTION RATE OF H₂S 0.1775 REACTION RATE OF SO₂ 0.0895

REACTION TEMPERATURE 510.00 REACTION PRESSURE 856.8

FEED H₂S/SO₂ RATIO 1.9327 PRODUCT H₂S/SO₂ RATIO 1.8937CONVERSION OF H₂S 44.99 CONVERSION OF SO₂ 43.85

MOLECULAR	FEED	PARTIAL PRESSURE	MATERIAL BALANCE	
SPECIE	COMPOSITION	IN REACTOR	FEED	PRODUCT
N ₂	95.22	818.7	14.510	14.510
H ₂ S	3.16	15.1	0.487	0.268
SO ₂	1.61	7.9	0.252	0.141
H ₂ O	0.00	12.4	0.000	0.221
SX	0.00	2.4	0.000	0.043
H ₂	0.00	0.0	0.000	-0.001

X=AVERAGE NUMBER OF ATOMS PER MOLECULE = 7.58197

GAMMA ALUMINA

WEIGHT OF CATALYST = 1.23520 (GRAMS)

RUN NUMBER 10

UNITS

MASS.....GRAM

PRESSURE.....MILLIMETERS OF MERCURY

TEMPERATURE.....DEGREES KELVIN

TIME.....HOUR

COMPOSITION.....MOLE PERCENT

VOLUME.....STANDARD CUBIC FEET

REACTION RATE...GM MOLES/(HR-GM OF CATALYST)

W/FH₂S (WEIGHT OF CATALYST/H₂S VOLUMETRIC FEED RATE) 3.553REACTION RATE OF H₂S 0.1684 REACTION RATE OF SO₂ 0.0848

REACTION TEMPERATURE 510.00 REACTION PRESSURE 856.8

FEED H₂S/SO₂ RATIO 1.9327 PRODUCT H₂S/SO₂ RATIO 1.8886CONVERSION OF H₂S 46.79 CONVERSION OF SO₂ 45.55

MOLECULAR	FEED	PARTIAL PRESSURE	MATERIAL BALANCE	
SPECIE	COMPOSITION	IN REACTOR	FEED	PRODUCT
N ₂	95.22	818.9	13.229	13.229
H ₂ S	3.16	14.6	0.444	0.236
SO ₂	1.61	7.7	0.229	0.125
H ₂ O	0.00	12.9	0.000	0.209
SX	0.00	2.5	0.000	0.041
H ₂	0.00	0.0	0.000	-0.001

X=AVERAGE NUMBER OF ATOMS PER MOLECULE = 7.57728

GAMMA ALUMINA

WEIGHT OF CATALYST = 1.23520 (GRAMS)

RUN NUMBER 11

UNITS

MASS.....GRAM

PRESSURE.....MILLIMETERS OF MERCURY

TEMPERATURE.....DEGREES KELVIN

TIME.....HOUR

COMPOSITION.....MOLE PERCENT

VOLUME.....STANDARD CUBIC FEET

REACTION RATE...GM MOLES/(HR-GM OF CATALYST)

W/FH₂S (WEIGHT OF CATALYST/H₂S VOLUMETRIC FEED RATE) 4.274REACTION RATE OF H₂S 0.1449 REACTION RATE OF SO₂ 0.0730

REACTION TEMPERATURE 510.00 REACTION PRESSURE 856.8

FEED H₂S/SO₂ RATIO 1.9327 PRODUCT H₂S/SO₂ RATIO 1.8869CONVERSION OF H₂S 48.46 CONVERSION OF SO₂ 47.21

MOLECULAR	FEED	PARTIAL PRESSURE	MATERIAL BALANCE	
SPECIE	COMPOSITION	IN REACTOR	FEED	PRODUCT
N ₂	95.22	819.0	10.997	10.997
H ₂ S	3.16	14.1	0.369	0.190
SO ₂	1.61	7.5	0.191	0.100
H ₂ O	0.00	13.4	0.000	0.180
SX	0.00	2.6	0.000	0.035
H ₂	0.00	0.0	0.000	-0.001

X=AVERAGE NUMBER OF ATOMS PER MOLECULE = 7.56395

GAMMA ALUMINA

WEIGHT OF CATALYST = 1.23520 (GRAMS)

RUN NUMBER 12

UNITS

MASS.....GRAM

PRESSURE.....MILLIMETERS OF MERCURY

TEMPERATURE.....DEGREES KELVIN

TIME.....HOUR

COMPOSITION.....MOLE PERCENT

VOLUME.....STANDARD CUBIC FEET

REACTION RATE...GM MOLES/(HR-GM OF CATALYST)

W/FH₂S (WEIGHT OF CATALYST/H₂S VOLUMETRIC FEED RATE) 5.355REACTION RATE OF H₂S 0.1220 REACTION RATE OF SO₂ 0.0615

REACTION TEMPERATURE 510.00 REACTION PRESSURE 856.8

FEED H₂S/SO₂ RATIO 1.9327 PRODUCT H₂S/SO₂ RATIO 1.8821CONVERSION OF H₂S 51.13 CONVERSION OF SO₂ 49.81

MOLECULAR	FEED	PARTIAL PRESSURE	MATERIAL BALANCE	
SPECIE	COMPOSITION	IN REACTOR	FEED	PRODUCT
N ₂	95.22	819.2	8.777	8.777
H ₂ S	3.16	13.4	0.294	0.144
SO ₂	1.61	7.1	0.152	0.076
H ₂ O	0.00	14.1	0.000	0.152
SX	0.00	2.8	0.000	0.030
H ₂	0.00	0.0	0.000	-0.001

X=AVERAGE NUMBER OF ATOMS PER MOLECULE = 7.54821

GAMMA ALUMINA

WEIGHT OF CATALYST = 1.23520 (GRAMS)

RUN NUMBER 13

UNITS

MASS.....GRAM

PRESSURE.....MILLIMETERS OF MERCURY

TEMPERATURE.....DEGREES KELVIN

TIME.....HOUR

COMPOSITION.....MOLE PERCENT

VOLUME.....STANDARD CUBIC FEET

REACTION RATE...GM MOLES/(HR-GM OF CATALYST)

W/FH₂S (WEIGHT OF CATALYST/H₂S VOLUMETRIC FEED RATE) 10.210REACTION RATE OF H₂S 0.0718 REACTION RATE OF SO₂ 0.0363

REACTION TEMPERATURE 510.00 REACTION PRESSURE 856.8

FEED H₂S/SO₂ RATIO 1.9327 PRODUCT H₂S/SO₂ RATIO 1.8785CONVERSION OF H₂S 57.38 CONVERSION OF SO₂ 56.15

MOLECULAR	FEED	PARTIAL PRESSURE	MATERIAL BALANCE	
SPECIE	COMPOSITION	IN REACTOR	FEED	PRODUCT
N ₂	95.22	819.6	4.604	4.604
H ₂ S	3.16	11.7	0.154	0.065
SO ₂	1.61	6.2	0.080	0.035
H ₂ O	0.00	16.0	0.000	0.089
SX	0.00	3.1	0.000	0.017
H ₂	0.00	0.0	0.000	-0.001

X=AVERAGE NUMBER OF ATOMS PER MOLECULE = 7.49696

GAMMA ALUMINA

WEIGHT OF CATALYST = 1.23520 (GRAMS)

RUN NUMBER 14

UNITS

MASS.....GRAM

PRESSURE.....MILLIMETERS OF MERCURY

TEMPERATURE.....DEGREES KELVIN

TIME.....HOUR

COMPOSITION.....MOLE PERCENT

VOLUME.....STANDARD CUBIC FEET

REACTION RATE...GM MOLES/(HR-GM OF CATALYST)

W/FH₂S (WEIGHT OF CATALYST/H₂S VOLUMETRIC FEED RATE) 2.394REACTION RATE OF H₂S 0.2417 REACTION RATE OF SO₂ 0.1201

REACTION TEMPERATURE 510.00 REACTION PRESSURE 856.8

FEED H₂S/SO₂ RATIO 1.9484 PRODUCT H₂S/SO₂ RATIO 1.8992CONVERSION OF H₂S 45.27 CONVERSION OF SO₂ 43.85

MOLECULAR	FEED	PARTIAL PRESSURE	MATERIAL BALANCE	
SPECIE	COMPOSITION	IN REACTOR	FEED	PRODUCT
N ₂	95.29	819.5	19.915	19.915
H ₂ S	3.11	14.8	0.659	0.360
SO ₂	1.58	7.8	0.338	0.190
H ₂ O	0.00	12.2	0.000	0.296
SX	0.00	2.4	0.000	0.058
H ₂	0.00	0.0	0.000	0.001

X=AVERAGE NUMBER OF ATOMS PER MOLECULE = 7.60779

2.0 PERCENT NAOH-DOPED GAMMA ALUMINA

WEIGHT OF CATALYST = 1.23520 (GRAMS)

RUN NUMBER 15

UNITS

MASS.....GRAM

PRESSURE.....MILLIMETERS OF MERCURY

TEMPERATURE.....DEGREES KELVIN

TIME.....HOUR

COMPOSITION.....MOLE PERCENT

VOLUME.....STANDARD CUBIC FEET

REACTION RATE...GM MOLES/(HR-GM OF CATALYST)

W/FH₂S (WEIGHT OF CATALYST/H₂S VOLUMETRIC FEED RATE) 2.919REACTION RATE OF H₂S 0.2196 REACTION RATE OF SO₂ 0.1089

REACTION TEMPERATURE 510.00 REACTION PRESSURE 856.8

FEED H₂S/SO₂ RATIO 1.9484 PRODUCT H₂S/SO₂ RATIO 1.8844CONVERSION OF H₂S 50.14 CONVERSION OF SO₂ 48.45

MOLECULAR	FEED	PARTIAL PRESSURE	MATERIAL BALANCE	
SPECIE	COMPOSITION	IN REACTOR	FEED	PRODUCT
N ₂	95.29	819.9	16.336	16.336
H ₂ S	3.11	13.5	0.541	0.269
SO ₂	1.58	7.1	0.277	0.143
H ₂ O	0.00	13.5	0.000	0.269
SX	0.00	2.6	0.000	0.053
H ₂	0.00	0.0	0.000	0.002

X=AVERAGE NUMBER OF ATOMS PER MOLECULE = 7.59971

2.0 PERCENT NaOH-DOPED GAMMA ALUMINA

WEIGHT OF CATALYST = 1.23520 (GRAMS)

RUN NUMBER 16

UNITS

MASS.....GRAM

PRESSURE.....MILLIMETERS OF MERCURY

TEMPERATURE.....DEGREES KELVIN

TIME.....HOUR

COMPOSITION.....MOLE PERCENT

VOLUME.....STANDARD CUBIC FEET

REACTION RATE...GM MOLES/(HR-GM OF CATALYST)

W/FH₂S (WEIGHT OF CATALYST/H₂S VOLUMETRIC FEED RATE) 3.283REACTION RATE OF H₂S 0.2088 REACTION RATE OF SO₂ 0.1040

REACTION TEMPERATURE 510.00 REACTION PRESSURE 856.8

FEED H₂S/SO₂ RATIO 1.9484 PRODUCT H₂S/SO₂ RATIO 1.8852CONVERSION OF H₂S 53.61 CONVERSION OF SO₂ 52.06

MOLECULAR	FEED	PARTIAL PRESSURE	MATERIAL BALANCE	
SPECIE	COMPOSITION	IN REACTOR	FEED	PRODUCT
N ₂	95.29	820.1	14.526	14.526
H ₂ S	3.11	12.5	0.481	0.223
SO ₂	1.58	6.6	0.246	0.118
H ₂ O	0.00	14.5	0.000	0.257
SX	0.00	2.8	0.000	0.050
H ₂	0.00	0.0	0.000	0.000

X=AVERAGE NUMBER OF ATOMS PER MOLECULE = 7.59557

2.0 PERCENT NAOH-DOPED GAMMA ALUMINA

WEIGHT OF CATALYST = 1.23520 (GRAMS)

RUN NUMBER 17

UNITS

MASS.....GRAM

PRESSURE.....MILLIMETERS OF MERCURY

TEMPERATURE.....DEGREES KELVIN

TIME.....HOUR

COMPOSITION.....MOLE PERCENT

VOLUME.....STANDARD CUBIC FEET

REACTION RATE...GM MOLES/(HR-GM OF CATALYST)

W/FH₂S (WEIGHT OF CATALYST/H₂S VOLUMETRIC FEED RATE) 3.601REACTION RATE OF H₂S 0.2005 REACTION RATE OF SO₂ 0.0998

REACTION TEMPERATURE 510.00 REACTION PRESSURE 856.8

FEED H₂S/SO₂ RATIO 1.9484 PRODUCT H₂S/SO₂ RATIO 1.8769CONVERSION OF H₂S 56.47 CONVERSION OF SO₂ 54.81

MOLECULAR	FEED	PARTIAL PRESSURE	MATERIAL BALANCE	
SPECIE	COMPOSITION	IN REACTOR	FEED	PRODUCT
N ₂	95.29	820.3	13.244	13.244
H ₂ S	3.11	11.8	0.438	0.190
SO ₂	1.58	6.3	0.225	0.101
H ₂ O	0.00	15.2	0.000	0.246
SX	0.00	3.0	0.000	0.048
H ₂	0.00	0.0	0.000	0.000

X=AVERAGE NUMBER OF ATOMS PER MOLECULE = 7.59211

2.0 PERCENT NaOH-DOPED GAMMA ALUMINA

WEIGHT OF CATALYST = 1.23520 (GRAMS)

RUN NUMBER 18

UNITS

MASS.....GRAM

PRESSURE.....MILLIMETERS OF MERCURY

TEMPERATURE.....DEGREES KELVIN

TIME.....HOUR

COMPOSITION.....MOLE PERCENT

VOLUME.....STANDARD CUBIC FEET

REACTION RATE...GM MOLES/(HR-GM OF CATALYST)

W/FH₂S (WEIGHT OF CATALYST/H₂S VOLUMETRIC FEED RATE) 4.332REACTION RATE OF H₂S 0.1740 REACTION RATE OF SO₂ 0.0859

REACTION TEMPERATURE 510.00 REACTION PRESSURE 856.8

FEED H₂S/SO₂ RATIO 1.9484 PRODUCT H₂S/SO₂ RATIO 1.8479CONVERSION OF H₂S 58.95 CONVERSION OF SO₂ 56.72

MOLECULAR	FEED	PARTIAL PRESSURE	MATERIAL BALANCE	
SPECIE	COMPOSITION	IN REACTOR	FEED	PRODUCT
N ₂	95.29	820.6	11.009	11.009
H ₂ S	3.11	11.1	0.364	0.149
SO ₂	1.58	6.0	0.187	0.080
H ₂ O	0.00	15.8	0.000	0.212
SX	0.00	3.1	0.000	0.042
H ₂	0.00	0.0	0.000	0.002

X=AVERAGE NUMBER OF ATOMS PER MOLECULE = 7.57958

2.0 PERCENT NAOH-DOPED GAMMA ALUMINA

WEIGHT OF CATALYST = 1.23520 (GRAMS)

RUN NUMBER 19

UNITS

MASS.....GRAM

PRESSURE.....MILLIMETERS OF MERCURY

TEMPERATURE.....DEGREES KELVIN

TIME.....HOUR

COMPOSITION.....MOLE PERCENT

VOLUME.....STANDARD CUBIC FEET

REACTION RATE...GM MOLES/(HR-GM OF CATALYST)

W/FH₂S (WEIGHT OF CATALYST/H₂S VOLUMETRIC FEED RATE) 5.427REACTION RATE OF H₂S 0.1487 REACTION RATE OF SO₂ 0.0744

REACTION TEMPERATURE 510.00 REACTION PRESSURE 856.8

FEED H₂S/SO₂ RATIO 1.9484 PRODUCT H₂S/SO₂ RATIO 1.8686CONVERSION OF H₂S 63.15 CONVERSION OF SO₂ 61.57

MOLECULAR	FEED	PARTIAL PRESSURE	MATERIAL BALANCE	
SPECIE	COMPOSITION	IN REACTOR	FEED	PRODUCT
N ₂	95.29	820.8	8.787	8.787
H ₂ S	3.11	10.0	0.291	0.107
SO ₂	1.58	5.3	0.149	0.057
H ₂ O	0.00	17.1	0.000	0.183
SX	0.00	3.4	0.000	0.036
H ₂	0.00	0.0	0.000	-0.000

X=AVERAGE NUMBER OF ATOMS PER MOLECULE = 7.56607

2.0 PERCENT NAOH-DOPED GAMMA ALUMINA

WEIGHT OF CATALYST = 1.23520 (GRAMS)

RUN NUMBER 20

UNITS

MASS.....GRAM

PRESSURE.....MILLIMETERS OF MERCURY

TEMPERATURE.....DEGREES KELVIN

TIME.....HOUR

COMPOSITION.....MOLE PERCENT

VOLUME.....STANDARD CUBIC FEET

REACTION RATE...GM MOLES/(HR-GM OF CATALYST)

W/FH₂S (WEIGHT OF CATALYST/H₂S VOLUMETRIC FEED RATE) 10.347REACTION RATE OF H₂S 0.0851 REACTION RATE OF SO₂ 0.0425

REACTION TEMPERATURE 510.00 REACTION PRESSURE 856.8

FEED H₂S/SO₂ RATIO 1.9484 PRODUCT H₂S/SO₂ RATIO 1.8462CONVERSION OF H₂S 68.87 CONVERSION OF SO₂ 67.15

MOLECULAR	FEED	PARTIAL PRESSURE	MATERIAL BALANCE	
SPECIE	COMPOSITION	IN REACTOR	FEED	PRODUCT
N ₂	95.29	821.2	4.609	4.609
H ₂ S	3.11	8.4	0.152	0.047
SO ₂	1.58	4.5	0.078	0.025
H ₂ O	0.00	18.7	0.000	0.105
SX	0.00	3.7	0.000	0.020
H ₂	0.00	0.0	0.000	-0.000

X=AVERAGE NUMBER OF ATOMS PER MOLECULE = 7.51346

2.0 PERCENT NAOH-DOPED GAMMA ALUMINA

WEIGHT OF CATALYST = 1.23520 (GRAMS)

RUN NUMBER 21

UNITS

MASS.....GRAM

PRESSURE.....MILLIMETERS OF MERCURY

TEMPERATURE.....DEGREES KELVIN

TIME.....HOUR

COMPOSITION.....MOLE PERCENT

VOLUME.....STANDARD CUBIC FEET

REACTION RATE...GM MOLES/(HR-GM OF CATALYST)

W/FH₂S (WEIGHT OF CATALYST/H₂S VOLUMETRIC FEED RATE) 10.552REACTION RATE OF H₂S 0.0819 REACTION RATE OF SO₂ 0.0409

REACTION TEMPERATURE 510.00 REACTION PRESSURE 856.8

FEED H₂S/SO₂ RATIO 1.9463 PRODUCT H₂S/SO₂ RATIO 1.8428CONVERSION OF H₂S 67.62 CONVERSION OF SO₂ 65.80

MOLECULAR	FEED	PARTIAL PRESSURE	MATERIAL BALANCE	
SPECIE	COMPOSITION	IN REACTOR	FEED	PRODUCT
N ₂	95.32	821.4	4.611	4.611
H ₂ S	3.09	8.7	0.151	0.049
SO ₂	1.57	4.7	0.077	0.026
H ₂ O	0.00	18.2	0.000	0.102
SX	0.00	3.6	0.000	0.020
H ₂	0.00	0.0	0.000	0.000

X=AVERAGE NUMBER OF ATOMS PER MOLECULE = 7.51098

5.0 PERCENT NAOH-DOPED GAMMA ALUMINA

WEIGHT OF CATALYST = 1.25150 (GRAMS)

RUN NUMBER 22

UNITS

MASS.....GRAM

PRESSURE.....MILLIMETERS OF MERCURY

TEMPERATURE.....DEGREES KELVIN

TIME.....HOUR

COMPOSITION.....MOLE PERCENT

VOLUME.....STANDARD CUBIC FEET

REACTION RATE...GM MOLES/(HR-GM OF CATALYST)

W/FH₂S (WEIGHT OF CATALYST/H₂S VOLUMETRIC FEED RATE) 5.534REACTION RATE OF H₂S 0.1424 REACTION RATE OF SO₂ 0.0714

REACTION TEMPERATURE 510.00 REACTION PRESSURE 856.8

FEED H₂S/SO₂ RATIO 1.9463 PRODUCT H₂S/SO₂ RATIO 1.8735CONVERSION OF H₂S 61.67 CONVERSION OF SO₂ 60.18

MOLECULAR	FEED	PARTIAL PRESSURE	MATERIAL BALANCE	
SPECIE	COMPOSITION	IN REACTOR	FEED	PRODUCT
N ₂	95.32	820.9	8.790	8.790
H ₂ S	3.09	10.3	0.289	0.110
SO ₂	1.57	5.5	0.148	0.059
H ₂ O	0.00	16.7	0.000	0.178
SX	0.00	3.3	0.000	0.035
H ₂	0.00	0.0	0.000	-0.000

X=AVERAGE NUMBER OF ATOMS PER MOLECULE = 7.56341

5.0 PERCENT NAOH-DOPED GAMMA ALUMINA

WEIGHT OF CATALYST = 1.25150 (GRAMS)

RUN NUMBER 23

UNITS

MASS.....GRAM

PRESSURE.....MILLIMETERS OF MERCURY

TEMPERATURE.....DEGREES KELVIN

TIME.....HOUR

COMPOSITION.....MOLE PERCENT

VOLUME.....STANDARD CUBIC FEET

REACTION RATE...GM MOLES/(HR-GM OF CATALYST)

W/FH ₂ S (WEIGHT OF CATALYST/H ₂ S VOLUMETRIC FEED RATE)	4.417
REACTION RATE OF H ₂ S 0.1659	REACTION RATE OF SO ₂ 0.0822
REACTION TEMPERATURE 510.00	REACTION PRESSURE 856.8
FEED H ₂ S/SO ₂ RATIO 1.9463	PRODUCT H ₂ S/SO ₂ RATIO 1.8579
CONVERSION OF H ₂ S 57.32	CONVERSION OF SO ₂ 55.30

MOLECULAR SPECIE	FEED COMPOSITION	PARTIAL PRESSURE IN REACTOR	MATERIAL BALANCE	
			FEED	PRODUCT
N ₂	95.32	820.7	11.014	11.014
H ₂ S	3.09	11.5	0.362	0.154
SO ₂	1.57	6.1	0.186	0.083
H ₂ O	0.00	15.3	0.000	0.205
SX	0.00	3.0	0.000	0.040
H ₂	0.00	0.0	0.000	0.001

X=AVERAGE NUMBER OF ATOMS PER MOLECULE = 7.57667

5.0 PERCENT NAOH-DOPED GAMMA ALUMINA

WEIGHT OF CATALYST = 1.25150 (GRAMS)

RUN NUMBER 24

UNITS

MASS.....GRAM

PRESSURE.....MILLIMETERS OF MERCURY

TEMPERATURE.....DEGREES KELVIN

TIME.....HOUR

COMPOSITION.....MOLE PERCENT

VOLUME.....STANDARD CUBIC FEET

REACTION RATE...GM MOLES/(HR-GM OF CATALYST)

W/FH₂S (WEIGHT OF CATALYST/H₂S VOLUMETRIC FEED RATE) 3.672REACTION RATE OF H₂S 0.1907 REACTION RATE OF SO₂ 0.0954

REACTION TEMPERATURE 510.00 REACTION PRESSURE 856.8

FEED H₂S/SO₂ RATIO 1.9463 PRODUCT H₂S/SO₂ RATIO 1.8882CONVERSION OF H₂S 54.76 CONVERSION OF SO₂ 53.37

MOLECULAR	FEED	PARTIAL PRESSURE	MATERIAL BALANCE	
SPECIE	COMPOSITION	IN REACTOR	FEED	PRODUCT
N ₂	95.32	820.4	13.249	13.249
H ₂ S	3.09	12.2	0.435	0.197
SO ₂	1.57	6.4	0.223	0.104
H ₂ O	0.00	14.8	0.000	0.239
SX	0.00	2.9	0.000	0.047
H ₂	0.00	0.0	0.000	-0.000

X=AVERAGE NUMBER OF ATOMS PER MOLECULE = 7.58907

5.0 PERCENT NAOH-DOPED GAMMA ALUMINA

WEIGHT OF CATALYST = 1.25150 (GRAMS)

RUN NUMBER 25

UNITS

MASS.....GRAM

PRESSURE.....MILLIMETERS OF MERCURY

TEMPERATURE.....DEGREES KELVIN

TIME.....HOUR

COMPOSITION.....MOLE PERCENT

VOLUME.....STANDARD CUBIC FEET

REACTION RATE...GM MOLES/(HR-GM OF CATALYST)

W/FH₂S (WEIGHT OF CATALYST/H₂S VOLUMETRIC FEED RATE) 3.348REACTION RATE OF H₂S 0.1977 REACTION RATE OF SO₂ 0.0993

REACTION TEMPERATURE 510.00 REACTION PRESSURE 856.8

FEED H₂S/SO₂ RATIO 1.9463 PRODUCT H₂S/SO₂ RATIO 1.9004CONVERSION OF H₂S 51.77 CONVERSION OF SO₂ 50.60

MOLECULAR	FEED	PARTIAL PRESSURE	MATERIAL BALANCE	
SPECIE	COMPOSITION	IN REACTOR	FEED	PRODUCT
N ₂	95.32	820.1	14.531	14.531
H ₂ S	3.09	13.0	0.477	0.230
SO ₂	1.57	6.8	0.245	0.121
H ₂ O	0.00	14.0	0.000	0.248
SX	0.00	2.7	0.000	0.048
H ₂	0.00	0.0	0.000	-0.001

X=AVERAGE NUMBER OF ATOMS PER MOLECULE = 7.59227

5.0 PERCENT NAOH-DOPED GAMMA ALUMINA

WEIGHT OF CATALYST = 1.25150 (GRAMS)

RUN NUMBER 26

UNITS

MASS.....GRAM

PRESSURE.....MILLIMETERS OF MERCURY

TEMPERATURE.....DEGREES KELVIN

TIME.....HOUR

COMPOSITION.....MOLE PERCENT

VOLUME.....STANDARD CUBIC FEET

REACTION RATE...GM MOLES/(HR-GM OF CATALYST)

W/FH₂S (WEIGHT OF CATALYST/H₂S VOLUMETRIC FEED RATE) 2.977REACTION RATE OF H₂S 0.2069 REACTION RATE OF SO₂ 0.1029

REACTION TEMPERATURE 510.00 REACTION PRESSURE 856.8

FEED H₂S/SO₂ RATIO 1.9463 PRODUCT H₂S/SO₂ RATIO 1.8902CONVERSION OF H₂S 48.17 CONVERSION OF SO₂ 46.64

MOLECULAR	FEED	PARTIAL PRESSURE	MATERIAL BALANCE	
SPECIE	COMPOSITION	IN REACTOR	FEED	PRODUCT
N ₂	95.32	819.9	16.343	16.343
H ₂ S	3.09	13.9	0.537	0.278
SO ₂	1.57	7.3	0.276	0.147
H ₂ O	0.00	12.9	0.000	0.257
SX	0.00	2.5	0.000	0.051
H ₂	0.00	0.0	0.000	0.001

X=AVERAGE NUMBER OF ATOMS PER MOLECULE = 7.59586

5.0 PERCENT NaOH-DOPED GAMMA ALUMINA

WEIGHT OF CATALYST = 1.25150 (GRAMS)

RUN NUMBER 27

UNITS

MASS.....GRAM

PRESSURE.....MILLIMETERS OF MERCURY

TEMPERATURE.....DEGREES KELVIN

TIME.....HOUR

COMPOSITION.....MOLE PERCENT

VOLUME.....STANDARD CUBIC FEET

REACTION RATE...GM MOLES/(HR-GM OF CATALYST)

W/FH₂S (WEIGHT OF CATALYST/H₂S VOLUMETRIC FEED RATE) 2.438REACTION RATE OF H₂S 0.2280 REACTION RATE OF SO₂ 0.1134

REACTION TEMPERATURE 510.00 REACTION PRESSURE 856.8

FEED H₂S/SO₂ RATIO 1.9463 PRODUCT H₂S/SO₂ RATIO 1.9002CONVERSION OF H₂S 43.49 CONVERSION OF SO₂ 42.12

MOLECULAR	FEED	PARTIAL PRESSURE	MATERIAL BALANCE	
SPECIE	COMPOSITION	IN REACTOR	FEED	PRODUCT
N ₂	95.32	819.5	19.952	19.952
H ₂ S	3.09	15.2	0.656	0.370
SO ₂	1.57	8.0	0.337	0.195
H ₂ O	0.00	11.6	0.000	0.284
SX	0.00	2.3	0.000	0.056
H ₂	0.00	0.0	0.000	0.001

X=AVERAGE NUMBER OF ATOMS PER MOLECULE = 7.60406

5.0 PERCENT NAOH-DOPED GAMMA ALUMINA

WEIGHT OF CATALYST = 1.25150 (GRAMS)

RUN NUMBER 28

UNITS

MASS.....GRAM

PRESSURE.....MILLIMETERS OF MERCURY

TEMPERATURE.....DEGREES KELVIN

TIME.....HOUR

COMPOSITION.....MOLE PERCENT

VOLUME.....STANDARD CUBIC FEET

REACTION RATE...GM MOLES/(HR-GM OF CATALYST)

W/FH₂S (WEIGHT OF CATALYST/H₂S VOLUMETRIC FEED RATE) 9.883REACTION RATE OF H₂S 0.0575 REACTION RATE OF SO₂ 0.0293

REACTION TEMPERATURE 510.00 REACTION PRESSURE 856.8

FEED H₂S/SO₂ RATIO 1.9365 PRODUCT H₂S/SO₂ RATIO 1.9180CONVERSION OF H₂S 44.46 CONVERSION OF SO₂ 43.92

MOLECULAR	FEED	PARTIAL PRESSURE	MATERIAL BALANCE	
SPECIE	COMPOSITION	IN REACTOR	FEED	PRODUCT
N ₂	95.05	817.3	4.594	4.594
H ₂ S	3.27	15.8	0.159	0.088
SO ₂	1.66	8.2	0.082	0.046
H ₂ O	0.00	12.9	0.000	0.072
SX	0.00	2.5	0.000	0.014
H ₂	0.00	0.0	0.000	-0.001

X=AVERAGE NUMBER OF ATOMS PER MOLECULE = 7.47445

BAUXITE

WEIGHT OF CATALYST = 1.23650 (GRAMS)

RUN NUMBER 29

UNITS

MASS.....GRAM

PRESSURE.....MILLIMETERS OF MERCURY

TEMPERATURE.....DEGREES KELVIN

TIME.....HOUR

COMPOSITION.....MOLE PERCENT

VOLUME.....STANDARD CUBIC FEET

REACTION RATE...GM MOLES/(HR-GM OF CATALYST)

W/FH₂S (WEIGHT OF CATALYST/H₂S VOLUMETRIC FEED RATE) 5.184REACTION RATE OF H₂S 0.0939 REACTION RATE OF SO₂ 0.0477

REACTION TEMPERATURE 510.00 REACTION PRESSURE 856.8

FEED H₂S/SO₂ RATIO 1.9365 PRODUCT H₂S/SO₂ RATIO 1.9186CONVERSION OF H₂S 38.08 CONVERSION OF SO₂ 37.50

MOLECULAR	FEED	PARTIAL PRESSURE	MATERIAL BALANCE	
SPECIE	COMPOSITION	IN REACTOR	FEED	PRODUCT
N ₂	95.05	816.8	8.758	8.758
H ₂ S	3.27	17.6	0.304	0.188
SO ₂	1.66	9.1	0.157	0.098
H ₂ O	0.00	11.0	0.000	0.118
SX	0.00	2.1	0.000	0.023
H ₂	0.00	0.0	0.000	-0.001

X=AVERAGE NUMBER OF ATOMS PER MOLECULE = 7.52373

BAUXITE

WEIGHT OF CATALYST = 1.23650 (GRAMS)

RUN NUMBER 30

UNITS

MASS.....GRAM

PRESSURE.....MILLIMETERS OF MERCURY

TEMPERATURE.....DEGREES KELVIN

TIME.....HOUR

COMPOSITION.....MOLE PERCENT

VOLUME.....STANDARD CUBIC FEET

REACTION RATE...GM MOLES/(HR-GM OF CATALYST)

W/FH₂S (WEIGHT OF CATALYST/H₂S VOLUMETRIC FEED RATE) 4.137REACTION RATE OF H₂S 0.1143 REACTION RATE OF SO₂ 0.0581

REACTION TEMPERATURE 510.00 REACTION PRESSURE 856.8

FEED H₂S/SO₂ RATIO 1.9365 PRODUCT H₂S/SO₂ RATIO 1.9202CONVERSION OF H₂S 36.99 CONVERSION OF SO₂ 36.46

MOLECULAR	FEED	PARTIAL PRESSURE	MATERIAL BALANCE	
SPECIE	COMPOSITION	IN REACTOR	FEED	PRODUCT
N ₂	95.05	816.7	10.974	10.974
H ₂ S	3.27	17.9	0.382	0.240
SO ₂	1.66	9.3	0.197	0.125
H ₂ O	0.00	10.7	0.000	0.143
SX	0.00	2.1	0.000	0.028
H ₂	0.00	0.0	0.000	-0.002

X=AVERAGE NUMBER OF ATOMS PER MOLECULE = 7.54248

BAUXITE

WEIGHT OF CATALYST = 1.23650 (GRAMS)

RUN NUMBER 31

UNITS

MASS.....GRAM

PRESSURE.....MILLIMETERS OF MERCURY

TEMPERATURE.....DEGREES KELVIN

TIME.....HOUR

COMPOSITION.....MOLE PERCENT

VOLUME.....STANDARD CUBIC FEET

REACTION RATE...GM MOLES/(HR-GM OF CATALYST)

W/FH₂S (WEIGHT OF CATALYST/H₂S VOLUMETRIC FEED RATE) 3.439REACTION RATE OF H₂S 0.1307 REACTION RATE OF SO₂ 0.0664

REACTION TEMPERATURE 510.00 REACTION PRESSURE 856.8

FEED H₂S/SO₂ RATIO 1.9365 PRODUCT H₂S/SO₂ RATIO 1.9209CONVERSION OF H₂S 35.15 CONVERSION OF SO₂ 34.63

MOLECULAR SPECIE	FEED COMPOSITION	PARTIAL PRESSURE IN REACTOR	MATERIAL BALANCE FEED	MATERIAL BALANCE PRODUCT
N ₂	95.05	816.6	13.201	13.201
H ₂ S	3.27	18.4	0.459	0.298
SO ₂	1.66	9.5	0.237	0.155
H ₂ O	0.00	10.1	0.000	0.164
SX	0.00	1.9	0.000	0.032
H ₂	0.00	0.0	0.000	-0.002

X=AVERAGE NUMBER OF ATOMS PER MOLECULE = 7.55489

BAUXITE

WEIGHT OF CATALYST = 1.23650 (GRAMS)

RUN NUMBER 32

UNITS

MASS.....GRAM

PRESSURE.....MILLIMETERS OF MERCURY

TEMPERATURE.....DEGREES KELVIN

TIME.....HOUR

COMPOSITION.....MOLE PERCENT

VOLUME.....STANDARD CUBIC FEET

REACTION RATE...GM MOLES/(HR-GM OF CATALYST)

W/FH₂S (WEIGHT OF CATALYST/H₂S VOLUMETRIC FEED RATE) 3.136REACTION RATE OF H₂S 0.1397 REACTION RATE OF SO₂ 0.0711

REACTION TEMPERATURE 510.00 REACTION PRESSURE 856.8

FEED H₂S/SO₂ RATIO 1.9365 PRODUCT H₂S/SO₂ RATIO 1.9227CONVERSION OF H₂S 34.26 CONVERSION OF SO₂ 33.79

MOLECULAR	FEED	PARTIAL PRESSURE	MATERIAL BALANCE	
SPECIE	COMPOSITION	IN REACTOR	FEED	PRODUCT
N ₂	95.05	816.5	14.479	14.479
H ₂ S	3.27	18.6	0.504	0.331
SO ₂	1.66	9.7	0.260	0.172
H ₂ O	0.00	9.9	0.000	0.175
SX	0.00	1.9	0.000	0.034
H ₂	0.00	0.0	0.000	-0.003

X=AVERAGE NUMBER OF ATOMS PER MOLECULE = 7.56102

BAUXITE

WEIGHT OF CATALYST = 1.23650 (GRAMS)

RUN NUMBER 33

UNITS

MASS.....GRAM

PRESSURE.....MILLIMETERS OF MERCURY

TEMPERATURE.....DEGREES KELVIN

TIME.....HOUR

COMPOSITION.....MOLE PERCENT

VOLUME.....STANDARD CUBIC FEET

REACTION RATE...GM MOLES/(HR-GM OF CATALYST)

W/FH₂S (WEIGHT OF CATALYST/H₂S VOLUMETRIC FEED RATE) 2.788REACTION RATE OF H₂S 0.1518 REACTION RATE OF SO₂ 0.0778

REACTION TEMPERATURE 510.00 REACTION PRESSURE 856.8

FEED H₂S/SO₂ RATIO 1.9365 PRODUCT H₂S/SO₂ RATIO 1.9296CONVERSION OF H₂S 33.10 CONVERSION OF SO₂ 32.86

MOLECULAR	FEED	PARTIAL PRESSURE	MATERIAL BALANCE	
SPECIE	COMPOSITION	IN REACTOR	FEED	PRODUCT
N ₂	95.05	816.4	16.283	16.283
H ₂ S	3.27	19.0	0.567	0.379
SO ₂	1.66	9.8	0.292	0.196
H ₂ O	0.00	9.6	0.000	0.192
SX	0.00	1.8	0.000	0.037
H ₂	0.00	0.0	0.000	-0.004

X=AVERAGE NUMBER OF ATOMS PER MOLECULE = 7.56870

BAUXITE

WEIGHT OF CATALYST = 1.23650 (GRAMS)

RUN NUMBER 34

UNITS

MASS.....GRAM

PRESSURE.....MILLIMETERS OF MERCURY

TEMPERATURE.....DEGREES KELVIN

TIME.....HOUR

COMPOSITION.....MOLE PERCENT

VOLUME.....STANDARD CUBIC FEET

REACTION RATE...GM MOLES/(HR-GM OF CATALYST)

W/FH₂S (WEIGHT OF CATALYST/H₂S VOLUMETRIC FEED RATE) 2.284REACTION RATE OF H₂S 0.1690 REACTION RATE OF SO₂ 0.0858

REACTION TEMPERATURE 510.00 REACTION PRESSURE 856.8

FEED H₂S/SO₂ RATIO 1.9365 PRODUCT H₂S/SO₂ RATIO 1.9227CONVERSION OF H₂S 30.19 CONVERSION OF SO₂ 29.69

MOLECULAR	FEED	PARTIAL PRESSURE	MATERIAL BALANCE	
SPECIE	COMPOSITION	IN REACTOR	FEED	PRODUCT
N ₂	95.05	816.2	19.879	19.879
H ₂ S	3.27	19.8	0.692	0.483
SO ₂	1.66	10.3	0.357	0.251
H ₂ O	0.00	8.7	0.000	0.212
SX	0.00	1.7	0.000	0.041
H ₂	0.00	0.0	0.000	-0.003

X=AVERAGE NUMBER OF ATOMS PER MOLECULE = 7.57795

BAUXITE

WEIGHT OF CATALYST = 1.23650 (GRAMS)

RUN NUMBER 35

UNITS

MASS.....GRAM

PRESSURE.....MILLIMETERS OF MERCURY

TEMPERATURE.....DEGREES KELVIN

TIME.....HOUR

COMPOSITION.....MOLE PERCENT

VOLUME.....STANDARD CUBIC FEET

REACTION RATE...GM MOLES/(HR-GM OF CATALYST)

W/FH ₂ S (WEIGHT OF CATALYST/H ₂ S VOLUMETRIC FEED RATE)	9.890
REACTION RATE OF H ₂ S 0.0708	REACTION RATE OF SO ₂ 0.0355
REACTION TEMPERATURE 510.00	REACTION PRESSURE 856.8
FEED H ₂ S/SO ₂ RATIO 1.9428	PRODUCT H ₂ S/SO ₂ RATIO 1.8871
CONVERSION OF H ₂ S 54.82	CONVERSION OF SO ₂ 53.48

MOLECULAR SPECIE	FEED COMPOSITION	PARTIAL PRESSURE IN REACTOR	MATERIAL BALANCE FEED	BALANCE PRODUCT
N ₂	95.06	818.3	4.594	4.594
H ₂ S	3.27	12.8	0.160	0.072
SO ₂	1.66	6.8	0.082	0.038
H ₂ O	0.00	15.6	0.000	0.088
SX	0.00	3.1	0.000	0.017
H ₂	0.00	0.0	0.000	-0.000

X=AVERAGE NUMBER OF ATOMS PER MOLECULE = 7.49548

2.0 PERCENT NAOH-DOPED BAUXITE

WEIGHT OF CATALYST = 1.23750 (GRAMS)

RUN NUMBER 36

UNITS

MASS.....GRAM

PRESSURE.....MILLIMETERS OF MERCURY

TEMPERATURE.....DEGREES KELVIN

TIME.....HOUR

COMPOSITION.....MOLE PERCENT

VOLUME.....STANDARD CUBIC FEET

REACTION RATE...GM MOLES/(HR-GM OF CATALYST)

W/FH ₂ S (WEIGHT OF CATALYST/H ₂ S VOLUMETRIC FEED RATE)	5.187
REACTION RATE OF H ₂ S 0.1180	REACTION RATE OF SO ₂ 0.0591
REACTION TEMPERATURE 510.00	REACTION PRESSURE 856.8
FEED H ₂ S/SO ₂ RATIO 1.9428	PRODUCT H ₂ S/SO ₂ RATIO 1.8959
CONVERSION OF H ₂ S 47.88	CONVERSION OF SO ₂ 46.59

MOLECULAR SPECIE	FEED COMPOSITION	PARTIAL PRESSURE IN REACTOR	MATERIAL BALANCE FEED	MATERIAL BALANCE PRODUCT
N ₂	95.06	817.7	8.759	8.759
H ₂ S	3.27	14.8	0.305	0.158
SO ₂	1.66	7.8	0.157	0.083
H ₂ O	0.00	13.6	0.000	0.146
SX	0.00	2.7	0.000	0.029
H ₂	0.00	0.0	0.000	-0.000

X=AVERAGE NUMBER OF ATOMS PER MOLECULE = 7.54504

2.0 PERCENT NAOH-DOPED BAUXITE

WEIGHT OF CATALYST = 1.23750 (GRAMS)

RUN NUMBER 37

UNITS

MASS.....GRAM

PRESSURE.....MILLIMETERS OF MERCURY

TEMPERATURE.....DEGREES KELVIN

TIME.....HOUR

COMPOSITION.....MOLE PERCENT

VOLUME.....STANDARD CUBIC FEET

REACTION RATE...GM MOLES/(HR-GM OF CATALYST)

W/FH₂S (WEIGHT OF CATALYST/H₂S VOLUMETRIC FEED RATE) 4.140REACTION RATE OF H₂S 0.1383 REACTION RATE OF SO₂ 0.0689

REACTION TEMPERATURE 510.00 REACTION PRESSURE 856.8

FEED H₂S/SO₂ RATIO 1.9428 PRODUCT H₂S/SO₂ RATIO 1.8944CONVERSION OF H₂S 44.80 CONVERSION OF SO₂ 43.39

MOLECULAR	FEED	PARTIAL PRESSURE	MATERIAL BALANCE	
SPECIE	COMPOSITION	IN REACTOR	FEED	PRODUCT
N ₂	95.06	817.5	10.974	10.974
H ₂ S	3.27	15.7	0.382	0.210
SO ₂	1.66	8.2	0.196	0.111
H ₂ O	0.00	12.7	0.000	0.170
SX	0.00	2.5	0.000	0.033
H ₂	0.00	0.0	0.000	0.000

X=AVERAGE NUMBER OF ATOMS PER MOLECULE = 7.55955

2.0 PERCENT NAOH-DOPED BAUXITE

WEIGHT OF CATALYST = 1.23750 (GRAMS)

RUN NUMBER 38

UNITS

MASS.....GRAM

PRESSURE.....MILLIMETERS OF MERCURY

TEMPERATURE.....DEGREES KELVIN

TIME.....HOUR

COMPOSITION.....MOLE PERCENT

VOLUME.....STANDARD CUBIC FEET

REACTION RATE...GM MOLES/(HR-GM OF CATALYST)

W/FH ₂ S (WEIGHT OF CATALYST/H ₂ S VOLUMETRIC FEED RATE)	3.442
REACTION RATE OF H ₂ S 0.1607	REACTION RATE OF SO ₂ 0.0801
REACTION TEMPERATURE 510.00	REACTION PRESSURE 856.8
FEED H ₂ S/SO ₂ RATIO 1.9428	PRODUCT H ₂ S/SO ₂ RATIO 1.8974
CONVERSION OF H ₂ S 43.27	CONVERSION OF SO ₂ 41.91

MOLECULAR SPECIE	FEED COMPOSITION	PARTIAL PRESSURE IN REACTOR	MATERIAL BALANCE FEED	MATERIAL BALANCE PRODUCT
N ₂	95.06	817.4	13.202	13.202
H ₂ S	3.27	16.1	0.459	0.260
SO ₂	1.66	8.5	0.236	0.137
H ₂ O	0.00	12.2	0.000	0.198
SX	0.00	2.4	0.000	0.039
H ₂	0.00	0.0	0.000	0.000

X=AVERAGE NUMBER OF ATOMS PER MOLECULE = 7.57303

2.0 (NAOH-DOPED BAUXITE

WEIGHT OF CATALYST = 1.23750 (GRAMS)

RUN NUMBER 39

UNITS

MASS.....GRAM

PRESSURE.....MILLIMETERS OF MERCURY

TEMPERATURE.....DEGREES KELVIN

TIME.....HOUR

COMPOSITION.....MOLE PERCENT

VOLUME.....STANDARD CUBIC FEET

REACTION RATE...GM MOLES/(HR-GM OF CATALYST)

W/FH₂S (WEIGHT OF CATALYST/H₂S VOLUMETRIC FEED RATE) 3.138REACTION RATE OF H₂S 0.1704 REACTION RATE OF SO₂ 0.0851

REACTION TEMPERATURE 510.00 REACTION PRESSURE 856.8

FEED H₂S/SO₂ RATIO 1.9428 PRODUCT H₂S/SO₂ RATIO 1.9021CONVERSION OF H₂S 41.83 CONVERSION OF SO₂ 40.59

MOLECULAR	FEED	PARTIAL PRESSURE	MATERIAL	BALANCE
SPECIE	COMPOSITION	IN REACTOR	FEED	PRODUCT
N ₂	95.06	817.3	14.480	14.480
H ₂ S	3.27	16.5	0.504	0.293
SO ₂	1.66	8.7	0.259	0.154
H ₂ O	0.00	11.8	0.000	0.210
SX	0.00	2.3	0.000	0.041
H ₂	0.00	0.0	0.000	0.000

X=AVERAGE NUMBER OF ATOMS PER MOLECULE = 7.57827

2.0 PERCENT NAOH-DOPED BAUXITE

WEIGHT OF CATALYST = 1.23750 (GRAMS)

RUN NUMBER 40

UNITS

MASS.....GRAM

PRESSURE.....MILLIMETERS OF MERCURY

TEMPERATURE.....DEGREES KELVIN

TIME.....HOUR

COMPOSITION.....MOLE PERCENT

VOLUME.....STANDARD CUBIC FEET

REACTION RATE...GM MOLES/(HR-GM OF CATALYST)

W/FH₂S (WEIGHT OF CATALYST/H₂S VOLUMETRIC FEED RATE) 2.790REACTION RATE OF H₂S 0.1755 REACTION RATE OF SO₂ 0.0876

REACTION TEMPERATURE 510.00 REACTION PRESSURE 856.8

FEED H₂S/SO₂ RATIO 1.9428 PRODUCT H₂S/SO₂ RATIO 1.9073CONVERSION OF H₂S 38.31 CONVERSION OF SO₂ 37.16

MOLECULAR	FEED	PARTIAL PRESSURE	MATERIAL BALANCE	
SPECIE	COMPOSITION	IN REACTOR	FEED	PRODUCT
N ₂	95.06	817.0	16.285	16.285
H ₂ S	3.27	17.5	0.567	0.349
SO ₂	1.66	9.2	0.291	0.183
H ₂ O	0.00	10.8	0.000	0.216
SX	0.00	2.1	0.000	0.042
H ₂	0.00	0.0	0.000	0.000

X=AVERAGE NUMBER OF ATOMS PER MOLECULE = 7.58084

2.0 PERCENT NAOH-DOPED BAUXITE

WEIGHT OF CATALYST = 1.23750 (GRAMS)

RUN NUMBER 41

UNITS

MASS.....GRAM

PRESSURE.....MILLIMETERS OF MERCURY

TEMPERATURE.....DEGREES KELVIN

TIME.....HOUR

COMPOSITION.....MOLE PERCENT

VOLUME.....STANDARD CUBIC FEET

REACTION RATE...GM MOLES/(HR-GM OF CATALYST)

W/FH₂S (WEIGHT OF CATALYST/H₂S VOLUMETRIC FEED RATE) 2.285REACTION RATE OF H₂S 0.1910 REACTION RATE OF SO₂ 0.0943

REACTION TEMPERATURE 510.00 REACTION PRESSURE 856.8

FEED H₂S/SO₂ RATIO 1.9428 PRODUCT H₂S/SO₂ RATIO 1.9028CONVERSION OF H₂S 34.15 CONVERSION OF SO₂ 32.77

MOLECULAR	FEED	PARTIAL PRESSURE	MATERIAL BALANCE	
SPECIE	COMPOSITION	IN REACTOR	FEED	PRODUCT
N ₂	95.06	816.7	19.881	19.881
H ₂ S	3.27	18.7	0.692	0.455
SO ₂	1.66	9.8	0.356	0.239
H ₂ O	0.00	9.5	0.000	0.233
SX	0.00	1.9	0.000	0.046
H ₂	0.00	0.0	0.000	0.002

X=AVERAGE NUMBER OF ATOMS PER MOLECULE = 7.58788

2.0 PERCENT NAOH-DOPED BAUXITE

WEIGHT OF CATALYST = 1.23750 (GRAMS)

RUN NUMBER 42

UNITS

MASS.....GRAM

PRESSURE.....MILLIMETERS OF MERCURY

TEMPERATURE.....DEGREES KELVIN

TIME.....HOUR

COMPOSITION.....MOLE PERCENT

VOLUME.....STANDARD CUBIC FEET

REACTION RATE...GM MOLES/(HR-GM OF CATALYST)

W/FH₂S (WEIGHT OF CATALYST/H₂S VOLUMETRIC FEED RATE) 10.536REACTION RATE OF H₂S 0.0290 REACTION RATE OF SO₂ 0.0138

REACTION TEMPERATURE 510.00 REACTION PRESSURE 856.8

FEED H₂S/SO₂ RATIO 1.9745 PRODUCT H₂S/SO₂ RATIO 1.9395CONVERSION OF H₂S 23.93 CONVERSION OF SO₂ 22.56

MOLECULAR	FEED	PARTIAL PRESSURE	MATERIAL BALANCE	
SPECIE	COMPOSITION	IN REACTOR	FEED	PRODUCT
N ₂	95.41	818.8	4.616	4.616
H ₂ S	3.05	20.1	0.149	0.113
SO ₂	1.53	10.4	0.075	0.058
H ₂ O	0.00	6.0	0.000	0.034
SX	0.00	1.2	0.000	0.007
H ₂	0.00	0.0	0.000	0.001

X=AVERAGE NUMBER OF ATOMS PER MOLECULE = 7.39635

H-Y ZEOLITE

WEIGHT OF CATALYST = 1.23350 (GRAMS)

RUN NUMBER 43

UNITS

MASS.....GRAM

PRESSURE.....MILLIMETERS OF MERCURY

TEMPERATURE.....DEGREES KELVIN

TIME.....HOUR

COMPOSITION.....MOLE PERCENT

VOLUME.....STANDARD CUBIC FEET

REACTION RATE...GM MOLES/(HR-GM OF CATALYST)

W/FH₂S (WEIGHT OF CATALYST/H₂S VOLUMETRIC FEED RATE) 5.581REACTION RATE OF H₂S 0.0386 REACTION RATE OF SO₂ 0.0194

REACTION TEMPERATURE 510.00 REACTION PRESSURE 856.8

FEED H₂S/SO₂ RATIO 1.9487 PRODUCT H₂S/SO₂ RATIO 1.9412CONVERSION OF H₂S 16.88 CONVERSION OF SO₂ 16.56

MOLECULAR	FEED	PARTIAL PRESSURE	MATERIAL BALANCE	
SPECIE	COMPOSITION	IN REACTOR	FEED	PRODUCT
N ₂	95.43	818.3	8.803	8.803
H ₂ S	3.02	21.8	0.282	0.234
SO ₂	1.53	11.2	0.145	0.120
H ₂ O	0.00	4.4	0.000	0.048
SX	0.00	0.8	0.000	0.009
H ₂	0.00	0.0	0.000	-0.000

X=AVERAGE NUMBER OF ATOMS PER MOLECULE = 7.43090

H-Y ZEOLITE

WEIGHT OF CATALYST = 1.23350 (GRAMS)

RUN NUMBER 44

UNITS

MASS.....GRAM

PRESSURE.....MILLIMETERS OF MERCURY

TEMPERATURE.....DEGREES KELVIN

TIME.....HOUR

COMPOSITION.....MOLE PERCENT

VOLUME.....STANDARD CUBIC FEET

REACTION RATE...GM MOLES/(HR-GM OF CATALYST)

W/FH₂S (WEIGHT OF CATALYST/H₂S VOLUMETRIC FEED RATE) 4.364REACTION RATE OF H₂S 0.0409 REACTION RATE OF SO₂ 0.0167

REACTION TEMPERATURE 510.00 REACTION PRESSURE 856.8

FEED H₂S/SO₂ RATIO 1.9788 PRODUCT H₂S/SO₂ RATIO 1.9187CONVERSION OF H₂S 13.98 CONVERSION OF SO₂ 11.28

MOLECULAR	FEED	PARTIAL PRESSURE	MATERIAL BALANCE	
SPECIE	COMPOSITION	IN REACTOR	FEED	PRODUCT
N ₂	95.36	817.9	11.020	11.020
H ₂ S	3.09	23.0	0.361	0.310
SO ₂	1.54	12.0	0.182	0.162
H ₂ O	0.00	3.0	0.000	0.041
SX	0.00	0.7	0.000	0.009
H ₂	0.00	0.0	0.000	0.009

X=AVERAGE NUMBER OF ATOMS PER MOLECULE = 7.42998

H-Y ZEOLITE

WEIGHT OF CATALYST = 1.23350 (GRAMS)

RUN NUMBER 45

UNITS

MASS.....GRAM

PRESSURE.....MILLIMETERS OF MERCURY

TEMPERATURE.....DEGREES KELVIN

TIME.....HOUR

COMPOSITION.....MOLE PERCENT

VOLUME.....STANDARD CUBIC FEET

REACTION RATE...GM MOLES/(HR-GM OF CATALYST)

W/FH₂S (WEIGHT OF CATALYST/H₂S VOLUMETRIC FEED RATE) 3.628REACTION RATE OF H₂S 0.0419 REACTION RATE OF SO₂ 0.0206

REACTION TEMPERATURE 510.00 REACTION PRESSURE -325.0

FEED H₂S/SO₂ RATIO 1.9788 PRODUCT H₂S/SO₂ RATIO 1.9716CONVERSION OF H₂S 11.91 CONVERSION OF SO₂ 11.58

MOLECULAR	FEED	PARTIAL PRESSURE	MATERIAL	BALANCE
SPECIE	COMPOSITION	IN REACTOR	FEED	PRODUCT
N ₂	95.36	-310.1	13.257	13.257
H ₂ S	3.09	-8.9	0.434	0.382
SO ₂	1.54	-4.5	0.219	0.194
H ₂ O	0.00	-1.1	0.000	0.050
SX	0.00	-0.2	0.000	0.010
H ₂	0.00	0.0	0.000	0.000

X=AVERAGE NUMBER OF ATOMS PER MOLECULE = 7.32471

H-Y ZEOLITE

WEIGHT OF CATALYST = 1.23350 (GRAMS)

RUN NUMBER 46

UNITS

MASS.....GRAM

PRESSURE.....MILLIMETERS OF MERCURY

TEMPERATURE.....DEGREES KELVIN

TIME.....HOUR

COMPOSITION.....MOLE PERCENT

VOLUME.....STANDARD CUBIC FEET

REACTION RATE...GM MOLES/(HR-GM OF CATALYST)

W/FH ₂ S (WEIGHT OF CATALYST/H ₂ S VOLUMETRIC FEED RATE)	3.308
REACTION RATE OF H ₂ S 0.0421	REACTION RATE OF SO ₂ 0.0182
REACTION TEMPERATURE 510.00	REACTION PRESSURE 856.8
FEED H ₂ S/SO ₂ RATIO 1.9788	PRODUCT H ₂ S/SO ₂ RATIO 1.9449
CONVERSION OF H ₂ S 10.90	CONVERSION OF SO ₂ 9.35

MOLECULAR SPECIE	FEED COMPOSITION	PARTIAL PRESSURE IN REACTOR	MATERIAL BALANCE FEED	MATERIAL BALANCE PRODUCT
N ₂	95.36	817.5	14.540	14.540
H ₂ S	3.09	23.8	0.476	0.424
SO ₂	1.54	12.2	0.240	0.218
H ₂ O	0.00	2.5	0.000	0.045
SX	0.00	0.5	0.000	0.010
H ₂	0.00	0.0	0.000	0.006

X=AVERAGE NUMBER OF ATOMS PER MOLECULE = 7.43514

H-Y ZEOLITE

WEIGHT OF CATALYST = 1.23350 (GRAMS)

RUN NUMBER 47

UNITS

MASS.....GRAM

PRESSURE.....MILLIMETERS OF MERCURY

TEMPERATURE.....DEGREES KELVIN

TIME.....HOUR

COMPOSITION.....MOLE PERCENT

VOLUME.....STANDARD CUBIC FEET

REACTION RATE...GM MOLES/(HR-GM OF CATALYST)

W/FH₂S (WEIGHT OF CATALYST/H₂S VOLUMETRIC FEED RATE) 2.941REACTION RATE OF H₂S 0.0433 REACTION RATE OF SO₂ 0.0196

REACTION TEMPERATURE 510.00 REACTION PRESSURE 856.8

FEED H₂S/SO₂ RATIO 1.9788 PRODUCT H₂S/SO₂ RATIO 1.9567CONVERSION OF H₂S 9.97 CONVERSION OF SO₂ 8.95

MOLECULAR	FEED	PARTIAL PRESSURE	MATERIAL BALANCE	
SPECIE	COMPOSITION	IN REACTOR	FEED	PRODUCT
N ₂	95.36	817.4	16.352	16.352
H ₂ S	3.09	24.1	0.536	0.482
SO ₂	1.54	12.3	0.270	0.246
H ₂ O	0.00	2.4	0.000	0.048
SX	0.00	0.5	0.000	0.010
H ₂	0.00	0.0	0.000	0.004

X=AVERAGE NUMBER OF ATOMS PER MOLECULE = 7.43977

H-Y ZEOLITE

WEIGHT OF CATALYST = 1.23350 (GRAMS)

RUN NUMBER 48

UNITS

MASS.....GRAM

PRESSURE.....MILLIMETERS OF MERCURY

TEMPERATURE.....DEGREES KELVIN

TIME.....HOUR

COMPOSITION.....MOLE PERCENT

VOLUME.....STANDARD CUBIC FEET

REACTION RATE...GM MOLES/(HR-GM OF CATALYST)

W/FH ₂ S (WEIGHT OF CATALYST/H ₂ S VOLUMETRIC FEED RATE)	2.409
REACTION RATE OF H ₂ S 0.0437	REACTION RATE OF SO ₂ 0.0173
REACTION TEMPERATURE 510.00	REACTION PRESSURE 856.8
FEED H ₂ S/SO ₂ RATIO 1.9788	PRODUCT H ₂ S/SO ₂ RATIO 1.9410
CONVERSION OF H ₂ S 8.24	CONVERSION OF SO ₂ 6.45

MOLECULAR SPECIE	FEED COMPOSITION	PARTIAL PRESSURE IN REACTOR	MATERIAL BALANCE	
			FEED	PRODUCT
N ₂	95.36	817.3	19.964	19.964
H ₂ S	3.09	24.5	0.654	0.600
SO ₂	1.54	12.6	0.330	0.309
H ₂ O	0.00	1.7	0.000	0.042
SX	0.00	0.4	0.000	0.010
H ₂	0.00	0.0	0.000	0.011

X=AVERAGE NUMBER OF ATOMS PER MOLECULE = 7.43631

H-Y ZEOLITE

WEIGHT OF CATALYST = 1.23350 (GRAMS)

RUN NUMBER 49

UNITS

MASS.....GRAM

PRESSURE.....MILLIMETERS OF MERCURY

TEMPERATURE.....DEGREES KELVIN

TIME.....HOUR

COMPOSITION.....MOLE PERCENT

VOLUME.....STANDARD CUBIC FEET

REACTION RATE...GM MOLES/(HR-GM OF CATALYST)

W/FH₂S (WEIGHT OF CATALYST/H₂S VOLUMETRIC FEED RATE) 10.464REACTION RATE OF H₂S 0.0310 REACTION RATE OF SO₂ 0.0143

REACTION TEMPERATURE 510.00 REACTION PRESSURE 856.8

FEED H₂S/SO₂ RATIO 1.9752 PRODUCT H₂S/SO₂ RATIO 1.9175CONVERSION OF H₂S 25.39 CONVERSION OF SO₂ 23.14

MOLECULAR	FEED	PARTIAL PRESSURE	MATERIAL BALANCE	
SPECIE	COMPOSITION	IN REACTOR	FEED	PRODUCT
N ₂	95.36	818.7	4.614	4.614
H ₂ S	3.08	20.0	0.151	0.112
SO ₂	1.54	10.4	0.076	0.058
H ₂ O	0.00	6.2	0.000	0.035
SX	0.00	1.3	0.000	0.007
H ₂	0.00	0.0	0.000	0.002

X=AVERAGE NUMBER OF ATOMS PER MOLECULE = 7.40303

NA-Y ZEOLITE

WEIGHT OF CATALYST = 1.23670 (GRAMS)

RUN NUMBER 50

UNITS

MASS.....GRAM

PRESSURE.....MILLIMETERS OF MERCURY

TEMPERATURE.....DEGREES KELVIN

TIME.....HOUR

COMPOSITION.....MOLE PERCENT

VOLUME.....STANDARD CUBIC FEET

REACTION RATE...GM MOLES/(HR-GM OF CATALYST)

W/FH ₂ S (WEIGHT OF CATALYST/H ₂ S VOLUMETRIC FEED RATE)	5.488
REACTION RATE OF H ₂ S 0.0469	REACTION RATE OF SO ₂ 0.0223
REACTION TEMPERATURE 510.00	REACTION PRESSURE 856.8
FEED H ₂ S/SO ₂ RATIO 1.9752	PRODUCT H ₂ S/SO ₂ RATIO 1.9453
CONVERSION OF H ₂ S 20.14	CONVERSION OF SO ₂ 18.91

MOLECULAR SPECIE	FEED COMPOSITION	PARTIAL PRESSURE IN REACTOR	MATERIAL BALANCE FEED	BALANCE PRODUCT
N ₂	95.36	818.2	8.796	8.796
H ₂ S	3.08	21.4	0.288	0.230
SO ₂	1.54	11.0	0.145	0.118
H ₂ O	0.00	5.1	0.000	0.055
SX	0.00	1.0	0.000	0.011
H ₂	0.00	0.0	0.000	0.002

X=AVERAGE NUMBER OF ATOMS PER MOLECULE = 7.45030

NA-Y ZEOLITE

WEIGHT OF CATALYST = 1.23670 (GRAMS)

RUN NUMBER 51

UNITS

MASS.....GRAM

PRESSURE.....MILLIMETERS OF MERCURY

TEMPERATURE.....DEGREES KELVIN

TIME.....HOUR

COMPOSITION.....MOLE PERCENT

VOLUME.....STANDARD CUBIC FEET

REACTION RATE...GM MOLES/(HR-GM OF CATALYST)

W/FH₂S (WEIGHT OF CATALYST/H₂S VOLUMETRIC FEED RATE) 4.380REACTION RATE OF H₂S 0.0531 REACTION RATE OF SO₂ 0.0253

REACTION TEMPERATURE 510.00 REACTION PRESSURE 856.8

FEED H₂S/SO₂ RATIO 1.9752 PRODUCT H₂S/SO₂ RATIO 1.9491CONVERSION OF H₂S 18.22 CONVERSION OF SO₂ 17.12

MOLECULAR	FEED	PARTIAL PRESSURE	MATERIAL BALANCE	
SPECIE	COMPOSITION	IN REACTOR	FEED	PRODUCT
N ₂	95.36	818.0	11.020	11.020
H ₂ S	3.08	21.9	0.360	0.295
SO ₂	1.54	11.2	0.182	0.151
H ₂ O	0.00	4.6	0.000	0.062
SX	0.00	0.9	0.000	0.013
H ₂	0.00	0.0	0.000	0.003

X=AVERAGE NUMBER OF ATOMS PER MOLECULE = 7.46375

NA-Y ZEOLITE

WEIGHT OF CATALYST = 1.23670 (GRAMS)

RUN NUMBER 52

UNITS

MASS.....GRAM

PRESSURE.....MILLIMETERS OF MERCURY

TEMPERATURE.....DEGREES KELVIN

TIME.....HOUR

COMPOSITION.....MOLE PERCENT

VOLUME.....STANDARD CUBIC FEET

REACTION RATE...GM MOLES/(HR-GM OF CATALYST)

W/FH₂S (WEIGHT OF CATALYST/H₂S VOLUMETRIC FEED RATE) 3.569REACTION RATE OF H₂S 0.0559 REACTION RATE OF SO₂ 0.0265

REACTION TEMPERATURE 510.00 REACTION PRESSURE 856.8

FEED H₂S/SO₂ RATIO 1.9770 PRODUCT H₂S/SO₂ RATIO 1.9545CONVERSION OF H₂S 15.60 CONVERSION OF SO₂ 14.63

MOLECULAR	FEED	PARTIAL PRESSURE	MATERIAL BALANCE	
SPECIE	COMPOSITION	IN REACTOR	FEED	PRODUCT
N ₂	95.27	817.0	13.240	13.240
H ₂ S	3.15	23.0	0.443	0.373
SO ₂	1.57	11.8	0.224	0.191
H ₂ O	0.00	4.0	0.000	0.065
SX	0.00	0.8	0.000	0.013
H ₂	0.00	0.0	0.000	0.003

X=AVERAGE NUMBER OF ATOMS PER MOLECULE = 7.46896

NA-Y ZEOLITE

WEIGHT OF CATALYST = 1.23670 (GRAMS)

RUN NUMBER 53

UNITS

MASS.....GRAM

PRESSURE.....MILLIMETERS OF MERCURY

TEMPERATURE.....DEGREES KELVIN

TIME.....HOUR

COMPOSITION.....MOLE PERCENT

VOLUME.....STANDARD CUBIC FEET

REACTION RATE...GM MOLES/(HR-GM OF CATALYST)

W/FH ₂ S (WEIGHT OF CATALYST/H ₂ S VOLUMETRIC FEED RATE)	3.254
REACTION RATE OF H ₂ S 0.0582	REACTION RATE OF SO ₂ 0.0277
REACTION TEMPERATURE 510.00	REACTION PRESSURE 856.8
FEED H ₂ S/SO ₂ RATIO 1.9770	PRODUCT H ₂ S/SO ₂ RATIO 1.9570
CONVERSION OF H ₂ S 14.82	CONVERSION OF SO ₂ 13.95

MOLECULAR SPECIE	FEED COMPOSITION	PARTIAL PRESSURE IN REACTOR	MATERIAL BALANCE FEED	MATERIAL BALANCE PRODUCT
N ₂	95.27	816.9	14.522	14.522
H ₂ S	3.15	23.2	0.485	0.413
SO ₂	1.57	11.8	0.245	0.211
H ₂ O	0.00	3.8	0.000	0.068
SX	0.00	0.8	0.000	0.014
H ₂	0.00	0.0	0.000	0.003

X=AVERAGE NUMBER OF ATOMS PER MOLECULE = 7.47341

NA-Y ZEOLITE

WEIGHT OF CATALYST = 1.23670 (GRAMS)

RUN NUMBER 54

UNITS

MASS.....GRAM

PRESSURE.....MILLIMETERS OF MERCURY

TEMPERATURE.....DEGREES KELVIN

TIME.....HOUR

COMPOSITION.....MOLE PERCENT

VOLUME.....STANDARD CUBIC FEET

REACTION RATE...GM MOLES/(HR-GM OF CATALYST)

W/FH ₂ S (WEIGHT OF CATALYST/H ₂ S VOLUMETRIC FEED RATE)	2.893
REACTION RATE OF H ₂ S 0.0608	REACTION RATE OF SO ₂ 0.0299
REACTION TEMPERATURE 510.00	REACTION PRESSURE 856.8
FEED H ₂ S/SO ₂ RATIO 1.9770	PRODUCT H ₂ S/SO ₂ RATIO 1.9684
CONVERSION OF H ₂ S 13.78	CONVERSION OF SO ₂ 13.40

MOLECULAR SPECIE	FEED COMPOSITION	PARTIAL PRESSURE IN REACTOR	MATERIAL BALANCE FEED	MATERIAL BALANCE PRODUCT
N ₂	95.27	816.8	16.332	16.332
H ₂ S	3.15	23.5	0.546	0.471
SO ₂	1.57	11.9	0.276	0.239
H ₂ O	0.00	3.7	0.000	0.074
SX	0.00	0.7	0.000	0.015
H ₂	0.00	0.0	0.000	0.001

X=AVERAGE NUMBER OF ATOMS PER MOLECULE = 7.47913

NA-Y ZEOLITE

WEIGHT OF CATALYST = 1.23670 (GRAMS)

RUN NUMBER 55

UNITS

MASS.....GRAM

PRESSURE.....MILLIMETERS OF MERCURY

TEMPERATURE.....DEGREES KELVIN

TIME.....HOUR

COMPOSITION.....MOLE PERCENT

VOLUME.....STANDARD CUBIC FEET

REACTION RATE...GM MOLES/(HR-GM OF CATALYST)

W/FH₂S (WEIGHT OF CATALYST/H₂S VOLUMETRIC FEED RATE) 2.370REACTION RATE OF H₂S 0.0550 REACTION RATE OF SO₂ 0.0264

REACTION TEMPERATURE 510.00 REACTION PRESSURE 856.8

FEED H₂S/SO₂ RATIO 1.9770 PRODUCT H₂S/SO₂ RATIO 1.9660CONVERSION OF H₂S 10.20 CONVERSION OF SO₂ 9.69

MOLECULAR SPECIE	FEED COMPOSITION	PARTIAL PRESSURE IN REACTOR	MATERIAL BALANCE	
			FEED	PRODUCT
N ₂	95.27	816.5	19.939	19.939
H ₂ S	3.15	24.5	0.667	0.599
SO ₂	1.57	12.4	0.337	0.304
H ₂ O	0.00	2.6	0.000	0.065
SX	0.00	0.5	0.000	0.013
H ₂	0.00	0.0	0.000	0.002

X=AVERAGE NUMBER OF ATOMS PER MOLECULE = 7.46774

NA-Y ZEOLITE

WEIGHT OF CATALYST = 1.23670 (GRAMS)

NOTE:

Run 6 was performed after the catalyst had been treated for 1 hour with a gaseous mixture of 1% CO₂ and 99% N₂

RUN NUMBER 4 (6.0 MIN. AFTER FEED INTRODUCED)
UNITS

MASS.....GRAM

PRESSURE.....MILLIMETERS OF MERCURY

TEMPERATURE.....DEGREES KELVIN

TIME.....HOUR

COMPOSITION.....MOLE PERCENT

VOLUME.....STANDARD CUBIC FEET

REACTION RATE...GM MOLES/(HR-GM OF CATALYST)

W/FCOS (WEIGHT OF CATALYST/COS VOLUMETRIC FEED RATE)	17.031
REACTION RATE OF COS 0.0419	REACTION RATE OF SO2 0.0203
REACTION TEMPERATURE 522.00	REACTION PRESSURE 856.8
FEED COS/SO2 RATIO 2.0514	PRODUCT COS/SO2 RATIO 2.0386
CONVERSION OF COS 56.55	CONVERSION OF SO2 56.28

MOLECULAR	FEED	PARTIAL PRESSURE	MATERIAL BALANCE	
SPECIE	COMPOSITION	IN REACTOR	FEED	PRODUCT
N2	93.09	804.2	3.960	3.960
CO2	-0.00	21.7	-0.000	0.107
COS	4.68	17.5	0.199	0.086
SO2	2.23	8.6	0.097	0.042
SX	0.00	4.5	0.000	0.022
ADSORBED				0.005

X=AVERAGE NUMBER OF ATOMS PER MOLECULE = 7.44830
GAMMA ALUMINA
WEIGHT OF CATALYST = 2.68420 (GRAMS)

RUN NUMBER 4 (24.0 MIN. AFTER FEED INTRODUCED)
UNITS

MASS.....GRAM

PRESSURE.....MILLIMETERS OF MERCURY

TEMPERATURE.....DEGREES KELVIN

TIME.....HOUR

COMPOSITION.....MOLE PERCENT

VOLUME.....STANDARD CUBIC FEET

REACTION RATE...GM MOLES/(HR-GM OF CATALYST)

W/FCOS (WEIGHT OF CATALYST/COS VOLUMETRIC FEED RATE)	17.031
REACTION RATE OF COS 0.0174	REACTION RATE OF SO2 0.0085
REACTION TEMPERATURE 522.00	REACTION PRESSURE 856.8
FEED COS/SO2 RATIO 2.0514	PRODUCT COS/SO2 RATIO 2.0540
CONVERSION OF COS 23.47	CONVERSION OF SO2 23.57

MOLECULAR SPECIE	FEED COMPOSITION	PARTIAL PRESSURE IN REACTOR	MATERIAL BALANCE FEED	BALANCE PRODUCT
N2	93.09	800.2	3.960	3.960
CO2	-0.00	8.8	-0.000	0.043
COS	4.68	30.8	0.199	0.152
SO2	2.23	14.9	0.097	0.074
SX	0.00	1.9	0.000	0.009
ADSORBED				0.002

X=AVERAGE NUMBER OF ATOMS PER MOLECULE = 7.34667
GAMMA ALUMINA
WEIGHT OF CATALYST = 2.68420 (GRAMS)

RUN NUMBER 4 (30.0 MIN. AFTER FEED INTRODUCED)
UNITS

MASS.....GRAM

PRESSURE.....MILLIMETERS OF MERCURY

TEMPERATURE.....DEGREES KELVIN

TIME.....HOUR

COMPOSITION.....MOLE PERCENT

VOLUME.....STANDARD CUBIC FEET

REACTION RATE...GM MOLES/(HR-GM OF CATALYST)

W/FCOS (WEIGHT OF CATALYST/COS VOLUMETRIC FEED RATE) 17.031

REACTION RATE OF COS 0.0119 REACTION RATE OF SO2 0.0057

REACTION TEMPERATURE 522.00 REACTION PRESSURE 856.8

FEED COS/SO2 RATIO 2.0514 PRODUCT COS/SO2 RATIO 2.0503

CONVERSION OF COS 16.06 CONVERSION OF SO2 16.02

MOLECULAR	FEED	PARTIAL PRESSURE	MATERIAL BALANCE
SPECIE	COMPOSITION	IN REACTOR	FEED PRODUCT
N2	93.09	799.2	3.960 3.960
CO2	-0.00	6.0	-0.000 0.030
COS	4.68	33.7	0.199 0.167
SO2	2.23	16.4	0.097 0.081
SX	0.00	1.3	0.000 0.006
ADSORBED			0.001

X=AVERAGE NUMBER OF ATOMS PER MOLECULE = 7.29834

GAMMA ALUMINA

WEIGHT OF CATALYST = 2.68420 (GRAMS)

RUN NUMBER 4 (36.0 MIN. AFTER FEED INTRODUCED)
UNITS

MASS.....GRAM

PRESSURE.....MILLIMETERS OF MERCURY

TEMPERATURE.....DEGREES KELVIN

TIME.....HOUR

COMPOSITION.....MOLE PERCENT

VOLUME.....STANDARD CUBIC FEET

REACTION RATE...GM MOLES/(HR-GM OF CATALYST)

W/FCOS (WEIGHT OF CATALYST/COS VOLUMETRIC FEED RATE)	17.031
REACTION RATE OF COS 0.0079	REACTION RATE OF SO2 0.0038
REACTION TEMPERATURE 522.00	REACTION PRESSURE 856.8
FEED COS/SO2 RATIO 2.0514	PRODUCT COS/SO2 RATIO 2.0485
CONVERSION OF COS 10.69	CONVERSION OF SO2 10.56

MOLECULAR SPECIE	FEED COMPOSITION	PARTIAL PRESSURE IN REACTOR	MATERIAL BALANCE FEED	MATERIAL BALANCE PRODUCT
N2	93.09	798.1	3.960	3.960
CO2	-0.00	4.4	-0.000	0.022
COS	4.68	35.8	0.199	0.177
SO2	2.23	17.5	0.097	0.086
SX	0.00	0.8	0.000	0.004
ADSORBED				-0.000

X=AVERAGE NUMBER OF ATOMS PER MOLECULE = 7.24347
GAMMA ALUMINA
WEIGHT OF CATALYST = 2.68420 (GRAMS)

RUN NUMBER 4 (54.0 MIN. AFTER FEED INTRODUCED)
UNITS

MASS.....GRAM

PRESSURE.....MILLIMETERS OF MERCURY

TEMPERATURE.....DEGREES KELVIN

TIME.....HOUR

COMPOSITION.....MOLE PERCENT

VOLUME.....STANDARD CUBIC FEET

REACTION RATE...GM MOLES/(HR-GM OF CATALYST)

W/FCOS (WEIGHT OF CATALYST/COS VOLUMETRIC FEED RATE)	17.031
REACTION RATE OF COS 0.0018	REACTION RATE OF SO2 0.0009
REACTION TEMPERATURE 522.00	REACTION PRESSURE 856.8
FEED COS/SO2 RATIO 2.0514	PRODUCT COS/SO2 RATIO 2.0522
CONVERSION OF COS 2.47	CONVERSION OF SO2 2.51

MOLECULAR	FEED	PARTIAL PRESSURE	MATERIAL BALANCE	
SPECIE	COMPOSITION	IN REACTOR	FEED	PRODUCT
N2	93.09	797.3	3.960	3.960
CO2	-0.00	1.0	-0.000	0.005
COS	4.68	39.1	0.199	0.194
SO2	2.23	19.0	0.097	0.094
SX	0.00	0.2	0.000	0.001
ADSORBED				-0.000

X=AVERAGE NUMBER OF ATOMS PER MOLECULE = 7.02266
GAMMA ALUMINA
WEIGHT OF CATALYST = 2.68420 (GRAMS)

RUN NUMBER 4 (60.0 MIN. AFTER FEED INTRODUCED)
UNITS

MASS.....GRAM

PRESSURE.....MILLIMETERS OF MERCURY

TEMPERATURE.....DEGREES KELVIN

TIME.....HOUR

COMPOSITION.....MOLE PERCENT

VOLUME.....STANDARD CUBIC FEET

REACTION RATE...GM MOLES/(HR-GM OF CATALYST)

W/FCOS (WEIGHT OF CATALYST/COS VOLUMETRIC FEED RATE)	17.031
REACTION RATE OF COS 0.0013	REACTION RATE OF SO2 0.0005
REACTION TEMPERATURE 522.00	REACTION PRESSURE 856.8
FEED COS/SO2 RATIO 2.0514	PRODUCT COS/SO2 RATIO 2.0483
CONVERSION OF COS 1.79	CONVERSION OF SO2 1.64

MOLECULAR	FEED	PARTIAL PRESSURE	MATERIAL BALANCE	
SPECIE	COMPOSITION	IN REACTOR	FEED	PRODUCT
N2	93.09	797.3	3.960	3.960
CO2	-0.00	0.7	-0.000	0.003
COS	4.68	39.3	0.199	0.195
SO2	2.23	19.2	0.097	0.095
SX	0.00	0.1	0.000	0.000
ADSORBED				-0.000

X=AVERAGE NUMBER OF ATOMS PER MOLECULE = 6.96187
GAMMA ALUMINA
WEIGHT OF CATALYST = 2.68420 (GRAMS)

RUN NUMBER 4 (66.0 MIN. AFTER FEED INTRODUCED)
UNITS

MASS.....GRAM

PRESSURE.....MILLIMETERS OF MERCURY

TEMPERATURE.....DEGREES KELVIN

TIME.....HOUR

COMPOSITION.....MOLE PERCENT

VOLUME.....STANDARD CUBIC FEET

REACTION RATE...GM MOLES/(HR-GM OF CATALYST)

W/FCOS (WEIGHT OF CATALYST/COS VOLUMETRIC FEED RATE) 17.031

REACTION RATE OF COS 0.0012 REACTION RATE OF SO2 0.0005

REACTION TEMPERATURE 522.00 REACTION PRESSURE 856.8

FEED COS/SO2 RATIO 2.0514 PRODUCT COS/SO2 RATIO 2.0495

CONVERSION OF COS 1.64 CONVERSION OF SO2 1.55

MOLECULAR	FEED	PARTIAL PRESSURE	MATERIAL	BALANCE
SPECIE	COMPOSITION	IN REACTOR	FEED	PRODUCT
N2	93.09	797.2	3.960	3.960
CO2	-0.00	0.7	-0.000	0.003
COS	4.68	39.4	0.199	0.195
SO2	2.23	19.2	0.097	0.095
SX	0.00	0.1	0.000	0.000
ADSORBED				-0.000

X=AVERAGE NUMBER OF ATOMS PER MOLECULE = 6.94744
GAMMA ALUMINA
WEIGHT OF CATALYST = 2.68420 (GRAMS)

RUN NUMBER 5 (6.0 MIN. AFTER FEED INTRODUCED)
UNITS

MASS.....GRAM

PRESSURE.....MILLIMETERS OF MERCURY

TEMPERATURE.....DEGREES KELVIN

TIME.....HOUR

COMPOSITION.....MOLE PERCENT

VOLUME.....STANDARD CUBIC FEET

REACTION RATE...GM MOLES/(HR-GM OF CATALYST)

W/FCOS (WEIGHT OF CATALYST/COS VOLUMETRIC FEED RATE) 25.906

REACTION RATE OF COS 0.0302 REACTION RATE OF SO2 0.0150

REACTION TEMPERATURE 557.00 REACTION PRESSURE 856.8

FEED COS/SO2 RATIO 2.0072 PRODUCT COS/SO2 RATIO 1.9990

CONVERSION OF COS 61.97 CONVERSION OF SO2 61.82

MOLECULAR	FEED	PARTIAL PRESSURE	MATERIAL BALANCE	
SPECIE	COMPOSITION	IN REACTOR	FEED	PRODUCT
N2	94.01	812.6	5.564	5.564
CO2	-0.00	19.8	-0.000	0.135
COS	4.02	13.2	0.238	0.090
SO2	1.96	6.6	0.118	0.045
SX	0.00	4.4	0.000	0.030
ADSORBED				0.012

X=AVERAGE NUMBER OF ATOMS PER MOLECULE = 7.25675

GAMMA ALUMINA

WEIGHT OF CATALYST = 4.88740 (GRAMS)

RUN NUMBER 5 (24.0 MIN. AFTER FEED INTRODUCED)
UNITS

MASS.....GRAM

PRESSURE.....MILLIMETERS OF MERCURY

TEMPERATURE.....DEGREES KELVIN

TIME.....HOUR

COMPOSITION.....MOLE PERCENT

VOLUME.....STANDARD CUBIC FEET

REACTION RATE...GM MOLES/(HR-GM OF CATALYST)

W/F_{CO}S (WEIGHT OF CATALYST/CO₂ VOLUMETRIC FEED RATE) 25.906

REACTION RATE OF CO₂ 0.0150 REACTION RATE OF SO₂ 0.0073

REACTION TEMPERATURE 557.00 REACTION PRESSURE 856.8

FEED CO₂/SO₂ RATIO 2.0072 PRODUCT CO₂/SO₂ RATIO 1.9895

CONVERSION OF CO₂ 30.75 CONVERSION OF SO₂ 30.13

MOLECULAR	FEED	PARTIAL PRESSURE	MATERIAL BALANCE	
SPECIE	COMPOSITION	IN REACTOR	FEED	PRODUCT
N ₂	94.01	809.0	5.564	5.564
CO ₂	-0.00	9.4	-0.000	0.065
CO ₂	4.02	24.0	0.238	0.165
SO ₂	1.96	12.0	0.118	0.083
SX	0.00	2.2	0.000	0.015
ADSORBED				0.008

X=AVERAGE NUMBER OF ATOMS PER MOLECULE = 7.15522

GAMMA ALUMINA

WEIGHT OF CATALYST = 4.88740 (GRAMS)

RUN NUMBER 5 (42.0 MIN. AFTER FEED INTRODUCED)
UNITS

MASS.....GRAM

PRESSURE.....MILLIMETERS OF MERCURY

TEMPERATURE.....DEGREES KELVIN

TIME.....HOUR

COMPOSITION.....MOLE PERCENT

VOLUME.....STANDARD CUBIC FEET

REACTION RATE...GM MOLES/(HR-GM OF CATALYST)

W/FCOS (WEIGHT OF CATALYST/COS VOLUMETRIC FEED RATE) 25.906

REACTION RATE OF COS 0.0049 REACTION RATE OF SO2 0.0024

REACTION TEMPERATURE 557.00 REACTION PRESSURE 856.8

FEED COS/SO2 RATIO 2.0072 PRODUCT COS/SO2 RATIO 2.0032

CONVERSION OF COS 10.07 CONVERSION OF SO2 9.90

MOLECULAR	FEED	PARTIAL PRESSURE	MATERIAL BALANCE	
SPECIE	COMPOSITION	IN REACTOR	FEED	PRODUCT
N2	94.01	806.3	5.564	5.564
CO2	-0.00	3.1	-0.000	0.021
COS	4.02	31.0	0.238	0.214
SO2	1.96	15.5	0.118	0.107
SX	0.00	0.7	0.000	0.005
ADSORBED				0.002

X=AVERAGE NUMBER OF ATOMS PER MOLECULE = 6.97241
GAMMA ALUMINA
WEIGHT OF CATALYST = 4.88740 (GRAMS)

RUN NUMBER 5 (54.0 MIN. AFTER FEED INTRODUCED)
UNITS

MASS.....GRAM

PRESSURE.....MILLIMETERS OF MERCURY

TEMPERATURE.....DEGREES KELVIN

TIME.....HOUR

COMPOSITION.....MOLE PERCENT

VOLUME.....STANDARD CUBIC FEET

REACTION RATE...GM MOLES/(HR-GM OF CATALYST)

W/FCOS (WEIGHT OF CATALYST/COS VOLUMETRIC FEED RATE) 25.906

REACTION RATE OF COS 0.0022 REACTION RATE OF SO2 0.0011

REACTION TEMPERATURE 557.00 REACTION PRESSURE 856.8

FEED COS/SO2 RATIO 2.0072 PRODUCT COS/SO2 RATIO 2.0064

CONVERSION OF COS 4.56 CONVERSION OF SO2 4.52

MOLECULAR	FEED	PARTIAL PRESSURE	MATERIAL BALANCE
SPECIE	COMPOSITION	IN REACTOR	FEED PRODUCT
N2	94.01	805.6	5.564 5.564
CO2	-0.00	1.4	-0.000 0.009
COS	4.02	32.9	0.238 0.227
SO2	1.96	16.4	0.118 0.113
SX	0.00	0.3	0.000 0.002
ADSORBED			0.000

X=AVERAGE NUMBER OF ATOMS PER MOLECULE = 6.82037

GAMMA ALUMINA

WEIGHT OF CATALYST = 4.88740 (GRAMS)

RUN NUMBER 5 (83.0 MIN. AFTER FEED INTRODUCED)
UNITS

MASS.....GRAM

PRESSURE.....MILLIMETERS OF MERCURY

TEMPERATURE.....DEGREES KELVIN

TIME.....HOUR

COMPOSITION.....MOLE PERCENT

VOLUME.....STANDARD CUBIC FEET

REACTION RATE...GM MOLES/(HR-GM OF CATALYST)

W/F_{COS} (WEIGHT OF CATALYST/COS VOLUMETRIC FEED RATE) 25.906

REACTION RATE OF COS 0.0007 REACTION RATE OF SO₂ 0.0003

REACTION TEMPERATURE 557.00 REACTION PRESSURE 856.8

FEED COS/SO₂ RATIO 2.0072 PRODUCT COS/SO₂ RATIO 2.0083

CONVERSION OF COS 1.56 CONVERSION OF SO₂ 1.61

MOLECULAR	FEED	PARTIAL PRESSURE	MATERIAL BALANCE
SPECIE	COMPOSITION	IN REACTOR	FEED PRODUCT
N ₂	94.01	805.3	5.564 5.564
CO ₂	-0.00	0.4	-0.000 0.003
COS	4.02	33.9	0.238 0.234
SO ₂	1.96	16.9	0.118 0.116
SX	0.00	0.1	0.000 0.000
ADSORBED			0.000

X=AVERAGE NUMBER OF ATOMS PER MOLECULE = 6.57454

GAMMA ALUMINA

WEIGHT OF CATALYST = 4.88740 (GRAMS)

RUN NUMBER 5 (96.0 MIN. AFTER FEED INTRODUCED)
UNITS

MASS.....GRAM

PRESSURE.....MILLIMETERS OF MERCURY

TEMPERATURE.....DEGREES KELVIN

TIME.....HOUR

COMPOSITION.....MOLE PERCENT

VOLUME.....STANDARD CUBIC FEET

REACTION RATE...GM MOLES/(HR-GM OF CATALYST)

W/FCOS (WEIGHT OF CATALYST/COS VOLUMETRIC FEED RATE) 25.906

REACTION RATE OF COS 0.0002 REACTION RATE OF SO2 0.0002

REACTION TEMPERATURE 557.00 REACTION PRESSURE 856.8

FEED COS/SO2 RATIO 2.0072 PRODUCT COS/SO2 RATIO 2.0162

CONVERSION OF COS 0.59 CONVERSION OF SO2 1.03

MOLECULAR	FEED	PARTIAL PRESSURE	MATERIAL BALANCE	
SPECIE	COMPOSITION	IN REACTOR	FEED	PRODUCT
N2	94.01	804.9	5.564	5.564
CO2	-0.00	0.4	-0.000	0.003
COS	4.02	34.2	0.238	0.237
SO2	1.96	17.0	0.118	0.117
SX	0.00	0.0	0.000	0.000
ADSORBED				-0.001

X=AVERAGE NUMBER OF ATOMS PER MOLECULE = 6.35088

GAMMA ALUMINA

WEIGHT OF CATALYST = 4.88740 (GRAMS)

RUN NUMBER 6 (12.0 MIN. AFTER FEED INTRODUCED)
UNITS

MASS.....GRAM

PRESSURE.....MILLIMETERS OF MERCURY

TEMPERATURE.....DEGREES KELVIN

TIME.....HOUR

COMPOSITION.....MOLE PERCENT

VOLUME.....STANDARD CUBIC FEET

REACTION RATE...GM MOLES/(HR-GM OF CATALYST)

W/FCOS (WEIGHT OF CATALYST/COS VOLUMETRIC FEED RATE)	10.205
REACTION RATE OF COS 0.0001	REACTION RATE OF SO2 0.0000
REACTION TEMPERATURE 510.00	REACTION PRESSURE 856.8
FEED COS/SO2 RATIO 2.0072	PRODUCT COS/SO2 RATIO 2.0065
CONVERSION OF COS 0.08	CONVERSION OF SO2 0.05

MOLECULAR SPECIE	FEED COMPOSITION	PARTIAL PRESSURE IN REACTOR	MATERIAL BALANCE	
			FEED	PRODUCT
N2	94.01	805.1	3.595	3.595
CO2	-0.00	-0.0	-0.000	-0.000
COS	4.02	34.4	0.154	0.153
SO2	1.96	17.1	0.076	0.076
SX	0.00	0.0	0.000	0.000
ADSORBED				0.000

X=AVERAGE NUMBER OF ATOMS PER MOLECULE = 6.33127
GAMMA ALUMINA
WEIGHT OF CATALYST = 1.24420 (GRAMS)

RUN NUMBER 6 (24.0 MIN. AFTER FEED INTRODUCED)
UNITS

MASS.....GRAM

PRESSURE.....MILLIMETERS OF MERCURY

TEMPERATURE.....DEGREES KELVIN

TIME.....HOUR

COMPOSITION.....MOLE PERCENT

VOLUME.....STANDARD CUBIC FEET

REACTION RATE...GM MOLES/(HR-GM OF CATALYST)

W/FCOS (WEIGHT OF CATALYST/COS VOLUMETRIC FEED RATE) 10.205

REACTION RATE OF COS-0.0001 REACTION RATE OF SO2 -0.0000

REACTION TEMPERATURE 510.00 REACTION PRESSURE 856.8

FEED COS/SO2 RATIO 2.0072 PRODUCT COS/SO2 RATIO 2.0079

CONVERSION OF COS -0.08 CONVERSION OF SO2 -0.05

MOLECULAR	FEED	PARTIAL PRESSURE	MATERIAL BALANCE
SPECIE	COMPOSITION	IN REACTOR	FEED PRODUCT
N2	94.01	805.0	3.595 3.595
CO2	-0.00	-0.0	-0.000 -0.000
COS	4.02	34.5	0.154 0.154
SO2	1.96	17.2	0.076 0.076
SX	0.00	-0.0	0.000 -0.000
ADSORBED			-0.000

X=AVERAGE NUMBER OF ATOMS PER MOLECULE = 6.33467
GAMMA ALUMINA
WEIGHT OF CATALYST = 1.24420 (GRAMS)

RUN NUMBER 6 (30.0 MIN. AFTER FEED INTRODUCED)
UNITS

MASS.....GRAM

PRESSURE.....MILLIMETERS OF MERCURY

TEMPERATURE.....DEGREES KELVIN

TIME.....HOUR

COMPOSITION.....MOLE PERCENT

VOLUME.....STANDARD CUBIC FEET

REACTION RATE...GM MOLES/(HR-GM OF CATALYST) .

W/F_{COS} (WEIGHT OF CATALYST/COS VOLUMETRIC FEED RATE) 10.205

REACTION RATE OF COS 0.0000 REACTION RATE OF SO₂ 0.0000

REACTION TEMPERATURE 510.00 REACTION PRESSURE 856.8

FEED COS/SO₂ RATIO 2.0072 PRODUCT COS/SO₂ RATIO 2.0072

CONVERSION OF COS 0.00 CONVERSION OF SO₂ 0.00

MOLECULAR	FEED	PARTIAL PRESSURE	MATERIAL BALANCE	
SPECIE	COMPOSITION	IN REACTOR	FEED	PRODUCT
N ₂	94.01	805.1	3.595	3.595
CO ₂	-0.00	-0.0	-0.000	-0.000
COS	4.02	34.5	0.154	0.154
SO ₂	1.96	17.1	0.076	0.076
SX	0.00	0.0	0.000	0.000
ADSORBED				0.000

X=AVERAGE NUMBER OF ATOMS PER MOLECULE = 2.00251
GAMMA ALUMINA
WEIGHT OF CATALYST = 1.24420 (GRAMS)

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